

(19) World Intellectual Property Organization
International Bureau



(43) International Publication Date
21 March 2002 (21.03.2002)

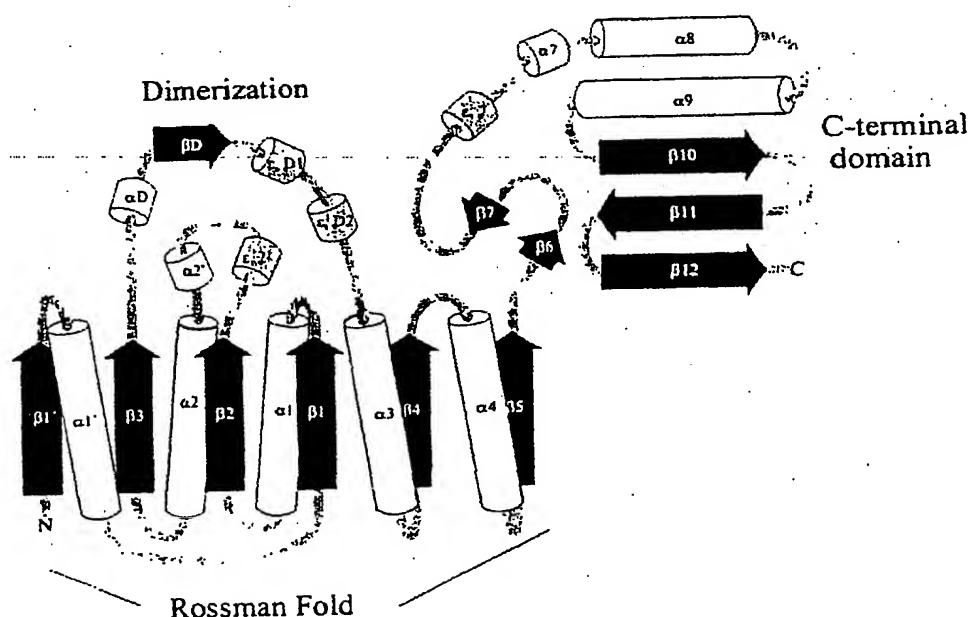
PCT

(10) International Publication Number
WO 02/22793 A1

- (51) International Patent Classification⁷: C12N 9/00, G06F 17/50
- (21) International Application Number: PCT/GB01/04067
- (22) International Filing Date:
11 September 2001 (11.09.2001)
- (25) Filing Language: English
- (26) Publication Language: English
- (30) Priority Data:
09/659,759 11 September 2000 (11.09.2000) US
- (63) Related by continuation (CON) or continuation-in-part (CIP) to earlier application:
US 09/659,759 (CIP)
Filed on 11 September 2000 (11.09.2000)
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- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW.
- (84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European

[Continued on next page]

(54) Title: CRYSTAL STRUCTURE OF PANTOTHENATE SYNTHETASE



(57) Abstract: A crystal of pantothenate synthetase (PS) has a monoclinic space group $P2_1$ and unit cell dimensions of $a = 66.0 \pm 0.2 \text{ \AA}$, $b = 78.1 \pm 0.2 \text{ \AA}$, $c = 77.1 \pm 0.2 \text{ \AA}$ and $\beta = 103.7 \pm 0.2^\circ$.



patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

— entirely in electronic form (except for this front page) and available upon request from the International Bureau

Published:

- with international search report
- before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

CRYSTAL STRUCTURE OF PANTOTHENATE SYNTHETASE

Field of the Invention

5 The present invention relates to the enzyme pantothenate synthetase, and in particular its crystal structure and the use of this structure in drug discovery.

Background of the Invention

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Pantothenic acid (vitamin B₅) is found in coenzyme A (CoA) and the acyl carrier protein (ACP), both of which are involved in fatty acid metabolism.

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Pantothenic acid can be synthesised by plants and microorganisms but animals are apparently unable to make the vitamin, and require it in their diet. However, all organisms are able to convert pantothenic acid to its metabolically active form, coenzyme A.

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The pathway for the synthesis of pantothenic acid is shown in Fig. 1. It provides a potential target for the treatment of infectious disease, since inhibitors of the pathway should be damaging to bacteria and fungi but not to human or animal

25

subjects infected by bacteria.

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Of specific interest is pantothenate synthetase (D-pantoate: β -alanine ligase (AMP-forming); EC 6.3.2.1). This enzyme catalyses the condensation between β -alanine and pantoic acid, the final steps in pantothenic acid biosynthesis. Inhibitors (whether competitive, non-competitive, uncompetitive or irreversible) of pantothenate synthetase would be of significant technical and commercial interest.

-2-

Purification of pantothenate synthetase (PS) to homogeneity was achieved by Miyatake et. al, (*J. Biochem.*, 79, (1976), 673-678). The enzyme was reported to require stoichiometric amounts of ATP as an energy source which is hydrolysed to AMP and inorganic pyrophosphate. The mechanism of the enzymic reaction involves pantoate adenylate as an intermediate.

However, until now no one has successfully determined the structure of PS. This has prevented PS inhibitors being developed via structure-based drug design methodologies. Knowledge of the structure of PS would significantly assist the rational design of novel therapeutics based on PS inhibitors.

Summary of the Invention

The present invention is at least partly based on overcoming several technical hurdles: we have (i) produced PS crystals of suitable quality, including crystals of selenium atom PS derivatives, for performing X-ray diffraction analyses, (ii) collected X-ray diffraction data from the crystals, (iii) determined a high resolution three-dimensional X-ray crystal structure of PS (i.e. a structure having a resolution which is numerically lower than 2 Å), and (iv) identified sites on the enzyme which are likely to be involved in the enzymic reaction.

In general aspects, the present invention is concerned with identifying or obtaining agent compounds (especially inhibitors of PS) for modulating PS activity, and in preferred embodiments identifying or obtaining actual agent compounds/inhibitors. Crystal structure information presented herein is useful in designing potential inhibitors and modelling them or their potential interaction with the PS

-3-

binding cavity. Potential inhibitors may be brought into contact with PS to test for ability to interact with the PS binding cavity. Actual inhibitors may be identified from among potential inhibitors synthesized following design and model work performed *in silico*. An inhibitor identified using the present invention may be formulated into a composition, for instance a composition comprising a pharmaceutically acceptable excipient, and may be used in the manufacture of a medicament for use in a method of treatment. These and other aspects and embodiments of the present invention are discussed below.

In a first aspect, the present invention provides a crystal of PS having a monoclinic space group $P2_1$, and unit cell dimensions of $a = 66.0 \pm 0.2 \text{ \AA}$, $b = 78.1 \pm 0.2 \text{ \AA}$, $c = 77.1 \pm 0.2 \text{ \AA}$ and $\beta = 103.7 \pm 0.2^\circ$. Preferably the PS is a dimer.

In a further aspect, the invention also provides a crystal of PS having the three dimensional atomic coordinates of Table 1. An advantageous feature of the structure defined by the atomic coordinates is that it has a high resolution, of about 1.7 \AA .

The coordinates of Table 1 provide a measure of atomic location in Angstroms, to a third decimal place. The coordinates are a relative set of positions that define a shape in three dimensions, but the skilled person would understand that an entirely different set of coordinates having a different origin and/or axes could define a similar or identical shape. Furthermore, the skilled person would understand that varying the relative atomic positions of the atoms of the structure so that the root mean square deviation of the residue backbone atoms (i.e. the nitrogen-carbon-carbon backbone atoms of the protein amino acid residues) is less than 1.5 \AA (preferably less than 1.0 \AA and more preferably

-4-

less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the residue backbone atoms, will generally result in a structure which is substantially the same as the structure of Table 1 in terms of both its structural characteristics and potency for structure-based design of PS inhibitors. Likewise the skilled person would understand that changing the number and/or positions of the water molecules and/or substrate molecules of Table 1 will not generally affect the potency of the structure for structure-based design of PS inhibitors. Thus for the purposes described herein as being aspects of the present invention, it is within the scope of the invention if: the Table 1 coordinates are transposed to a different origin and/or axes; the relative atomic positions of the atoms of the structure are varied so that the root mean square deviation of residue backbone atoms is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the residue backbone atoms; and/or the number and/or positions of water molecules and/or substrate molecules is varied. Reference herein to the coordinate data of Table 1 thus includes the coordinate data in which one or more individual values of the Table are varied in this way. By "root mean square deviation" we mean the square root of the arithmetic mean of the squares of the deviations from the mean.

Thus, for example, varying the atomic positions of the atoms of the structure by up to about 0.2 Å in any direction will result in a structure which is substantially the same as the structure of Table 1 in terms of both its structural characteristics and utility e.g. for structure-based drug design.

The provision of the high resolution structure of Table 1

-5-

provides those of skill in the art with a detailed insight into the mechanisms of action of PS. This insight provides a means to design new antibacterial agents which have the potential to inhibit the process of pantothenate synthesis in bacteria and fungi, or to modulate the activity of the enzyme, for example such that the enzyme works more effectively on prodrugs which are converted by PS into an antibacterial drug.

In a further aspect, the invention provides a method for crystallizing a selenium atom PS derivative which comprises producing PS by recombinant production in a bacterial host (e.g. *E.coli*) in the presence of selenomethionine, recovering a selenium atom PS derivative from the host and growing crystals from the recovered selenium atom PS derivative.

Thus, the selenium atom PS derivative and PS produced by crystallising native PS (see the detailed description below) are provided as crystallised proteins suitable for X-ray diffraction analysis.

The crystals may be grown by any suitable method, e.g. the hanging drop method.

The above aspects of the invention, both singly and in combination, all contribute to features of the invention which are advantageous.

The provision of the crystal structure of PS allows a novel approach for drug discovery for modulators of this enzyme. Accordingly, the invention provides a computer-based method of rational drug design which comprises:

providing the structure of the PS as defined by the coordinates of Table 1;

providing the structure of a candidate modulator molecule;

-6-

and

fitting the structure of the candidate modulator molecule to the structure of the PS of Table 1.

5 In an alternative aspect, the method of the invention may utilise the coordinates of atoms of interest of the PS which are in the vicinity of a putative substrate and/or co-factor binding regions in order to model the pocket in which the substrate or co-factor binds. These coordinates may be used to define a space which is
10 then screened "*in silico*" against a candidate modulator molecule. Thus the invention provides a computer-based method of rational drug design which comprises:

providing the coordinates of at least two atoms of the PS of Table 1 ("selected coordinates");

15 providing the structure of a candidate modulator molecule; and

fitting the structure of the candidate modulator molecule to the selected coordinates of the PS.

20 In practice, it will be desirable to model a sufficient number of atoms of the PS as defined by the coordinates of Table 1 which represent a binding pocket. Binding pockets and other features of the interaction of PS with co-factor are described in the detailed description. Thus, in this embodiment of the invention,
25 there will preferably be provided the coordinates of at least 5, preferably at least 10, more preferably at least 50 and even more preferably at least 100 selected atoms of the PS structure.

Our structure of PS has allowed us to identify particular sites
30 of interaction of Mg^{2+} , ATP, pantoate and β -alanine. The selected coordinates preferably include at least one of the coordinates defining these particular sites. Residues providing some of these sites include Pro28, Met30, His34, Asp35, Gly36, His37, Leu40, Asn58, Gln61, Phe62, Tyr71, Arg123, His126, Ile133,

-7-

Vall134, Leu137, Lys151, Gln155, Met178, Ala185, Leu186, Ser187, Ser188, and Arg189.

As discussed in the detailed description, we believe that ATP
5 interacts with one or more of Met30, His34, Asp35, Gly36, His37, Leu40, Lys151, Met178, Ala185, Leu186, Ser187, Ser188, and Arg189; Mg^{2+} interacts with either or both of Tyr71 and Ser188; pantoate interacts with one or more of Pro28, Met30, Asn58, Gln61, Ile133, Vall134, Leu137, and Gln155; and β -alanine
10 interacts with one or more of Met30, Phe62, Tyr71, Arg123, and His126.

In another aspect, the method of the invention may utilise a sub-domain of interest of the PS which is in the vicinity of a region
15 which binds substrate or co-factor. Thus, the invention provides a computer-based method of rational drug design which comprises:
providing the coordinates of at least a sub-domain of the PS;
providing the structure of a candidate modulator molecule;
20 and
fitting the structure of the candidate modulator molecule to the coordinates of the PS sub-domain provided.

Brief Description of the Drawings

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Fig. 1 shows schematically the pathway for the synthesis of pantothenic acid,

Figs. 2a-c show the general structure of PS, being respectively (a) a "cartoon" of the dimer, (b) a schematic
30 diagram of the monomer topology with numbering of secondary structures, and (c) a schematic plot of hydrogen bonding patterns between secondary structures,
Fig. 3 is a stereo pair of images showing schematically the core of the dimerisation interface, and

-8-

Fig. 4 shows a Connolly surface generated around the proposed PS active sites.

Detailed Description of the Invention

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By "fitting", it is meant determining by automatic, or semi-automatic means, interactions between at least one atom of the candidate and at least one atom of the PS, and calculating the extent to which such an interaction is stable. Interactions include attraction and repulsion, brought about by charge, steric considerations and the like. Various computer-based methods for fitting are described further herein.

By "sub-domain" is meant at least one (e.g. one, two, three or four) complete element(s) of secondary structure, i.e. an alpha helix or a beta sheet, as described in the detailed description below.

Table 1 gives atomic coordinate data for PS (which we have crystallised as a dimer) and associated water molecules. In Table 1 "Atom type" refers to the respective element, the first letter defining the element; "X, Y, Z" define, with respect to the crystallographic axes, the atomic position (in Å) of the respective atom; "Occ." is the occupancy of the atom in the respective position; and "B" is a temperature factor (in Å²) which accounts for movement of the atom around its atomic centre.

Particular regions of the PS include those identified as putative substrate or cofactor binding regions based on the data provided in Table 1.

As indicated above, modulators of PS may be inhibitors of the enzyme or compounds which affect its specificity or activity in relation to pantoate in other ways. The invention is

-9-

particularly suitable for the design, screening and development of PS inhibitor components. It is thus a preferred aspect of the invention that modulators are inhibitors.

5

The step of providing the structure of a candidate modulator molecule may involve selecting the compound by computationally screening a database of compounds for interaction with the active site. For example, a 3-D descriptor for the potential modulator may be derived, the descriptor including geometric and functional constraints derived from the architecture and chemical nature of the active site. The descriptor may then be used to interrogate the compound database, a potential modulator being a compound that has a good match to the features of the descriptor. In effect, the descriptor is a type of virtual pharmacophore.

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In any event, the determination of the three-dimensional structure of PS provides a basis for the design of new and specific ligands for PS. For example, knowing the three-dimensional structure of PS, computer modelling programs may be used to design different molecules expected to interact with possible or confirmed active sites, such as binding sites or other structural or functional features of PS.

25

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More specifically, a potential modulator of PS activity can be examined through the use of computer modelling using a docking program such as GRAM, DOCK, or AUTODOCK (see Walters et al., *Drug Discovery Today*, Vol.3, No.4, (1998), 160-178, and Dunbrack et al., *Folding and Design*, 2, (1997), 27-42) to identify potential inhibitors of PS. This procedure can include computer fitting of potential inhibitors to PS to ascertain how well the shape and the chemical structure of the potential inhibitor will bind to the enzyme.

-10-

Also computer-assisted, manual examination of the active site structure of PS may be performed. The use of programs such as GRID (Goodford, *J. Med. Chem.*, 28, (1985), 849-857) - a
5 program that determines probable interaction sites between molecules with various functional groups and the enzyme surface - may also be used to analyse the active site to predict partial structures of inhibiting compounds.

10 Computer programs can be employed to estimate the attraction, repulsion, and steric hindrance of the two binding partners (e.g. the PS and a potential inhibitor). Generally the tighter the fit, the fewer the steric hindrances; and the greater the attractive forces, the more potent the potential
15 modulator, since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug, the more likely it is that the drug will not interact with other proteins as well. This will tend to minimise potential side-effects due to unwanted
20 interactions with other proteins.

In a further aspect, the present invention provides a method for identifying a candidate modulator (e.g. potential inhibitor) of PS comprising the steps of:

25 employing a three-dimensional structure of PS, or at least one sub-domain thereof, to characterise at least one PS active site, the three-dimensional structure being defined by atomic coordinate data according to Table 1; and
identifying the candidate modulator by designing or
30 selecting a compound for interaction with the active site.

If more than one PS active site is characterised and a plurality of respective compounds are designed or selected, the modulator may be formed by linking the respective compounds

-11-

into a larger compound which maintains the relative positions and orientations of the respective compounds at the active sites. The larger compound may be formed as a real molecule or by computer modelling.

5

The step of identifying the candidate modulator may involve selecting the compound by computationally screening a database of compounds for interaction with the active site.

10

In another aspect, in place of *in silico* methods, high throughput screening of compounds to select compounds with binding activity may be undertaken, and those compounds which show binding activity may be selected as possible candidate modulators, and further crystallized with PS (e.g. by co-

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crystallization or by soaking) for X-ray analysis. The resulting X-ray structure may be compared with that of Table 1 for a variety of purposes. For example, where the contacts made by such compounds overlap with those made by pantoate, novel molecules comprising residues which contain contacts of both pantoate and the other compound may be provided.

20

Having designed or selected possible binding candidate modulators by determining those which have favourable fitting properties (e.g. strong attraction between candidate and PS), these can then be screened for activity. Consequently, the method preferably further comprises the steps of:

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obtaining or synthesising the candidate modulator; and contacting the candidate modulator with PS to determine the ability of the candidate modulator to interact with PS.

30

More preferably, in the latter step the candidate modulator is contacted with PS under conditions to determine its function.

For example, in the contacting step above the candidate

-12-

modulator is contacted with PS in the presence of a substrate, and typically a buffer, to determine the ability of said candidate modulator to inhibit PS. The substrate may be e.g. pantoic acid (or a salt thereof), β -alanine (or a salt thereof), or ATP. So, for example, an assay mixture for PS
5 may be produced which comprises the candidate modulator, substrate and buffer.

10 Instead of, or in addition to, performing such an assay, the method may comprise the further steps of:
obtaining or synthesising said candidate modulator;
forming a complex of PS and said candidate modulator; and
analysing said complex by X-ray crystallography to
15 determine the ability of said candidate modulator to interact with PS. Detailed structural information can then be obtained about the binding of the candidate modulator to PS, and in the light of this information adjustments can be made to the structure or functionality of the candidate modulator, e.g. to improve binding to the active site. The above steps may be
20 repeated and re-repeated as necessary.

In another aspect, the invention relates to a method of determining three dimensional structures of PS homologues of unknown structure by utilising the structural coordinates of
25 Table 1.

For example, if X-ray crystallographic or NMR spectroscopic data is provided for a PS homologue of unknown structure, the structure of PS as defined by Table 1 may be used to interpret
30 that data to provide a likely structure for the PS homologue by techniques which are well known in the art, e.g. phase modelling in the case of X-ray crystallography.

One embodiment of the method comprises the steps of:

-13-

(a) aligning a representation of an amino acid sequence of a PS homologue of unknown structure with the amino acid sequence of PS to match homologous regions of the amino acid sequences;

5 (b) modelling the structure of the matched homologous regions of the PS of unknown structure on the structure as defined by Table 1 of the corresponding regions of PS; and

10 (c) determining a conformation (e.g. so that favourable interactions are formed within the PS of unknown structure and/or so that a low energy conformation is formed) for the PS of unknown structure which substantially preserves the structure of said matched homologous regions.

15 The term "homologous regions" describes amino acid residues in two sequences that are identical or have similar (e.g. aliphatic, aromatic, polar, negatively charged, or positively charged) side-chain chemical groups. Identical and similar residues in homologous regions are sometimes described as being respectively "invariant" and "conserved" by those
20 skilled in the art.

Preferably one or all of steps (a) to (c) are performed by computer modelling. Homology modelling is a technique that is well known to those skilled in the art (see e.g. Greer,
25 *Science*, Vol. 228, (1985), 1055, and Blundell et al., *Eur. J. Biochem*, Vol. 172, (1988), 513).

30 In general, comparison of amino acid sequences is accomplished by aligning the amino acid sequence of a polypeptide of a known structure with the amino acid sequence of the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous are grouped together. This method detects conserved regions of the polypeptides and accounts for amino

-14-

acid insertions or deletions.

Homology between amino acid sequences can be determined using commercially available algorithms. The programs *BLAST*, *gapped*
5 *BLAST*, *BLASTN* and *PSI-BLAST* (provided by the National Center for Biotechnology Information) are widely used in the art for this purpose, and can align homologous regions of two amino acid sequences.

- 10 Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in a computer representation of the polypeptide with known structure are transferred to the
15 corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.
- 20 The structures of amino acids located in non-conserved regions may be assigned manually by using standard peptide geometries or by molecular simulation techniques, such as molecular
25 dynamics. The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or energy minimization.

The aspects of the invention described herein which utilise the PS structure *in silico* may be equally applied to homologue models of PS obtained by the above aspect of the invention,
30 and this application forms a further aspect of the present invention. Thus having determined a conformation of a PS by the method described above, such a conformation may be used in a computer-based method of rational drug design as described herein.

-15-

In another aspect, the invention includes a compound which is identified as a modulator (preferably an inhibitor) of PS by the methods of the invention described above.

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Following identification of an inhibitor compound, it may be manufactured and/or used in the preparation, i.e. manufacture or formulation, of a composition such as a medicament, pharmaceutical composition or drug. These may be administered to individuals.

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Thus, the present invention extends in various aspects not only to an inhibitor as provided by the invention, but also a pharmaceutical composition, medicament, drug or other composition comprising such an inhibitor e.g. for treatment (which may include preventative treatment) of disease such as microbial infection; a method comprising administration of such a composition to a patient, e.g. for treatment of disease such as microbial infection; use of such an inhibitor in the manufacture of a composition for administration, e.g. for treatment of disease such as microbial infection; and a method of making a pharmaceutical composition comprising admixing such an inhibitor with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

25

In a further aspect, the invention provides a method for determining the structure of a modulator of PS bound to PS, said method comprising:

30

providing a crystal of PS according to the invention; soaking the crystal with said modulator; and determining the structure of said PS-modulator complex.

Alternatively, the PS and modulator may be co-crystallized.

-16-

In either case, pantoate, β -alanine and/or pantothenate or an analogue thereof may optionally be present.

Having obtained and characterized a modulator compound
5 according to the invention, the invention further provides a method for modulating the activity of PS which method comprises:

providing PS under conditions where, in the absence of modulator, the PS is able to synthesize pantothenate from
10 pantoate;

providing a modulator compound; and

determining the extent to which the activity of PS is altered by the presence of said compound.

15 In another aspect, the present invention provides systems, particularly a computer system, intended to generate structures and/or perform rational drug design for PS or a complex of PS and a potential modulator, the systems containing either (a) atomic coordinate data according to
20 Table 1, said data defining the three-dimensional structure of PS or at least one sub-domain thereof, or (b) structure factor data for PS, said structure factor data being derivable from the atomic coordinate data of Table 1.

25 In a further aspect, the present invention provides computer readable media with either (a) atomic coordinate data according to Table 1 recorded thereon, said data defining the three-dimensional structure of PS, at least one atom or at
30 least one sub-domain thereof, or (b) structure factor data for PS recorded thereon, the structure factor data being derivable from the atomic coordinate data of Table 1.

As used herein, "computer readable media" refers to any medium or media which can be read and accessed directly by a

-17-

computer. Such media include, but are not limited to:
magnetic storage media such as floppy discs, hard disc storage
medium and magnetic tape; optical storage media such as
optical discs or CD-ROM; electrical storage media such as RAM
5 and ROM; and hybrids of these categories such as
magnetic/optical storage media.

By providing such computer readable media, the atomic
coordinate data can be routinely accessed to model PS or a
10 sub-domain thereof. For example, RASMOL (Sayle et al., *TIBS*,
Vol. 20, (1995), 374) is a publicly available computer
software package which allows access and analysis of atomic
coordinate data for structure determination and/or rational
drug design.

15 On the other hand, structure factor data, which are derivable
from atomic coordinate data (see e.g. Blundell et al., in
Protein Crystallography, Academic Press, New York, London and
San Francisco, (1976)), are particularly useful for
20 calculating e.g. difference Fourier electron density maps.

As used herein, "a computer system" refers to the hardware
means, software means and data storage means used to analyse
the atomic coordinate data of the present invention. The
25 minimum hardware means of the computer-based systems of the
present invention comprises a central processing unit (CPU),
input means, output means and data storage means. Desirably a
monitor is provided to visualise structure data. The data
storage means may be RAM or means for accessing computer
30 readable media of the sixth aspect of the invention. Examples
of such systems are microcomputer workstations available from
Silicon Graphics Incorporated and Sun Microsystems running
Unix based, Windows NT or IBM OS/2 operating systems.

-18-

In a further aspect, the invention provides a method of analysing a complex of PS and a potential modulator comprising the step of employing (i) X-ray crystallographic diffraction data from the complex and (ii) a three-dimensional structure of PS, or at least one sub-domain thereof, to generate a difference Fourier electron density map of the complex, the three-dimensional structure being defined by atomic coordinate data according to Table 1. The difference Fourier electron density map may then be analysed.

Therefore, such complexes can be crystallised and analysed using X-ray diffraction methods, e.g. according to the approach described by Greer et al., *J. of Medicinal Chemistry*, Vol. 37, (1994), 1035-1054, and difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallised PS and the solved structure of uncomplexed PS. These maps can then be analysed e.g. to determine whether and where a particular ligand binds to PS and/or changes the conformation of PS.

Electron density maps can be calculated using programs such as those from the CCP4 computing package (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763.). For map visualisation and model building programs such as "O" (Jones et al., *Acta Crystallography*, A47, (1991), 110-119) can be used.

PS Structural Characterization

We have found that the structure of a PS monomer consists of two major domains, joined at about residue 176 (Figs. 2a-c). Domain N (so called because it contains the N terminal) has an alpha-beta-alpha architecture; six parallel β -strands with 1'-

-19-

3-2-1-4-5 topology alternate with α -helices to form a Rossman fold with central β -sheet sandwiched between two layers of α -helices (Fig. 2b). The helices ($\alpha 1'$, 1, 2, 3 and 4) pack against the β -sheet in a right-handed way. The secondary structural elements have been numbered in Figs. 2a and b, with elements that are insertions or additions to the "standard" nucleotide-binding Rossman fold (discussed below under "Identification of Likely Active Sites") denoted by primes. Strand $\beta 5$ leads directly into the short β -hairpin and 3_{10} helix motif ($\beta 6$, $\beta 7$ and ϵ_{107}), which lies at the head of domain C (containing the C terminal) and is likely to be involved in phosphate binding (see below). The rest of the domain has a simple two-layer organisation: a helix-turn-helix layered above a flat sheet of three anti-parallel β -strands ($\alpha 8$ and 9 , $\beta 10$ -12). This sheet faces a prominent cleft in domain N, the predicted catalytic region (see below), making the whole structure resemble somewhat a pot (domain N) with its lid (domain C) on a hinge, a common arrangement in two-domain enzymes.

20

We have also found that the two monomers, A and B, of PS are related by a non-crystallographic quasi 2-fold rotational symmetry (NCS) axis. The dimerisation interface has a surface area of 1340 \AA^2 and the core of the interface is shown in Fig.

25

3. The centre of the nearly symmetrical dimerisation interface is unusual: below a 2-strand β -sheet (βD from A and B) Val109, Met166 and Phe168 form a hydrophobic pocket around weakly H-bonded polar clusters of Ser135, conserved Asn139 and three water molecules, one of which lies on the NCS axis.

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Above the β -sheet Tyr108, Asp110 and Arg128 form a tight charged cluster, and the rest of the interface consists of salt bridges (His106 to Asp165; Arg11 to Asp169) and extensive water-mediated H-bonding interactions.

-20-

The average B-factor of monomer B is about 4 Å² greater than that of A, which on the whole contains fewer disordered stretches. Also conformational differences between the monomers which can be explained by crystal packing
5 arrangements are found at residues 173-180 and 187-193.

For residues B187-193, electron density was poor, and the apparent backbone connectivity could not be reconciled with stereochemical and Ramachandran constraints. The loop was
10 eventually modelled using the same residues from monomer A (which are well ordered), and transformed by the operation that superimposes domain C of monomer A onto monomer B. However, it is likely that residues A187-193 are only ordered because the bottom of the dimerisation region is
15 crystallographically packed tightly against this region and that the disordered seen in B is more realistic for the apo-enzyme *in vivo*.

Residues 239-244 also have entirely different but defined
20 backbone conformations in the two monomers, and this difference is not readily explained by crystal packing. However, there appears to be no functional significance in the anomaly.

25 *Solving the PS Crystal Structure*

To solve the PS crystal structure, molecular replacement was not possible because prior to our determination of the PS structure similarities between the amino acid sequence of
30 *E.coli* PS and that of proteins with known structures were not evident. Therefore, phase information needed to be obtained *ab initio*.

The phase problem was first approached by the Multiple

-21-

Isomorphous Replacement technique, and crystals of PS were soaked with a range of heavy atom salts at a range of concentrations. However, the majority of these conditions resulted in crystal damage.

5

Eventually, production of selenomethionine PS (SeMet PS) was attempted, the selenium atoms being introduced into the protein prior to crystallisation by recombinant production of the protein in the presence of L-selenomethionine. This was successfully accomplished and is discussed in more detail below. X-ray analysis was performed on PS and SeMet PS crystals.

10

1. Production and purification of PS

15

Native PS

DNA encoding the PanC gene was engineered into a pUC19 expression vector. *E.coli* cells were transformed using the plasmid.

20

Colonies of transformed cells were inoculated directly into LB medium containing ampicillin (100 mg/ml) and IPTG (70mg/ml); induction of expression was continuous. The cultures were shaken (200 rpm on an orbital shaker) overnight at 37°C, when the cells were retrieved by centrifugation of the culture medium and the cell pellet stored frozen at -80°C.

25

Selenomethionine PS

30

The same *E.coli* strain was used as for native expression, but the methionine pathway inhibition system (see van Duyne et al., *J. Mol. Biol.*, 229, (1993), 105-124) was used for selenomethionine incorporation. Cells were grown on a

-22-

minimal, defined medium (see Table 2) containing selenomethionine as well as six other amino acids, whose presence inhibits the natural pathways for methionine synthesis. A starter culture (100ml) of the same medium as
5 above, but without selenomethionine or the inhibitory amino acids, was inoculated with transformed cells and grown at 37°C to log growth phase. 1ml of this culture was used to inoculate baffled 2/Erlemeyer flasks (250ml complete medium per flask) which were shaken at 37°C overnight and harvested as
10 for native protein.

Purification

Harvested cells were suspended in 20-40ml TD buffer (50mM
15 Tris/HCl pH 7.5 + 0.1mM dithiothreitol) sonicated at maximum intensity for 8 times 15 seconds, with 15 second breaks, and cell debris removed by centrifugation (30 minutes, 15000x g).

The supernatant was stirred at 4°C while (NH₄)₂SO₄ was added
20 slowly over ca. 15 minutes to a final concentration of 29.1% (w/v); after a further 30 minutes of stirring, precipitated contaminants were removed by centrifugation (30 minutes, 15000x g). The solution was dialysed overnight against TD
buffer (at least 2l).

The dialysed protein solution was loaded at 4°C onto an anion
exchange column (Pharmacia Q-Sepharose, 16/10) and eluted with
TD buffer against a NaCl gradient of 0 to 500mM in 75 minutes,
at a flow rate of 5ml/min. The protein eluted between 0.21
30 and 0.24M NaCl. The protein-containing fractions were selected from SDS-PAGE analysis, and concentrated to ca 1ml.

The concentrated fractions were loaded at 4°C onto a size
exclusion column (Pharmacia S200HR), and eluted with TD buffer

-23-

containing NaCl at 500mM. The fractions containing PS were confirmed by SDS-PAGE analysis. The fractions were pooled and dialysed overnight against TD buffer (at least 2l).

5 The dialysed protein solution was loaded at room temperature onto an affinity column (Pharmacia Blue Sepharose HiLoad 16/10) and eluted with at least five column volumes of TD buffer containing 10mM ATP. This effectively eluted all the protein, although this was not monitored directly.

10

ATP was removed from the eluant by repeated cycles (at least 5) of concentration (in a stirred cell concentrator (Amicon7 Ultrafiltration Cell) under pressure in an N₂ atmosphere) and dilution with TD buffer; ATP content was monitored by the UV spectrum (220-300nm) of the solution. The protein was finally concentrated (Ultrafree7 concentrator) to a concentration of between 20 and 30 mg/ml. At this concentration, the solution could be aliquoted and frozen directly at -80°C without damage to the protein.

20

For the purification of the SeMet protein, some precautions were taken to minimise oxidation of the selenium in the protein. The DTT concentration in all buffers was raised to 5mM, all buffers were thoroughly purged with N₂ gas before use, and the whole procedure was completed as fast as possible, within two days. The SeMet preparations of PS were subjected to Electrospray Mass Spectrometry (ESMS) to confirm the incorporation of selenomethionine during the expression.

25

30 2. Preparation of Crystals.

Crystals of PS and SeMet PS were grown using the hanging drop vapour diffusion method. Protein (20mg/ml) was mixed on a 1:1 ratio with crystallisation solution containing 4-7% (w/w)

-24-

Polyethylene Glycol 4000 and 50mM Tris/HCl buffer at pH8. Crystals formed within 2-4 days at 19°C. Crystallisation of SeMet PS, was performed using a nearly identical protocol, but additionally, 2mM DTT was added to the crystallisation solution before mixing the drop.

Crystals ideally have approximate dimensions of 600x200x50 µm. Under non-optimal conditions, crystals grow in clusters and are generally much thinner in the 3rd dimension (10-20 µm).

Crystals of PS were cryo-protected using a protocol of gradual soaking in the cryo-protectant, glycerol. A crystal was placed in 20ul of crystallisation solution, and the concentration of glycerol is gradually increased to 28% (v/v) in 4% increments.

3. Structural Determination

Multi-wavelength data sets were collected from a cryo-cooled crystal of SeMet PS, on beam line X-25 of the NSLS at Brookhaven National Laboratories on Long Island, USA. This is a high-flux station with good intensity and wavelength stability. The presence of selenomethionine in the protein was confirmed independently by electrospray mass spectrometry. Before the experiment, a large number of crystals were extensively screened for highest resolution, low mosaicity and low background scatter.

Terminal radiation-induced diffraction decay was evident in the first crystal to be exposed, which influenced data collection from the second, final SeMet crystal.

In addition to the three data sets collected from SeMet crystals, a data set was collected from a large native

-25-

crystal, which had been established to be nearly isomorphous with the SeMet crystals used. In order to have complete but also high resolution data, the same oscillation range was exposed twice, the first for measuring low resolution data (i.e. short exposures), and the second for the highest resolution possible (long exposures). All data were processed using MOSFLM (Leslie, *Joint CCP4 and EESF-EACMB Newsletter on Protein Crystallography*, Vol.26, Daresbury Laboratory, UK) and scaled with SCALA (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763).

The selenium atoms were located using the program SnB (Weeks et al., *J. of Applied Crystallography*, 32, (1999), 120-124) and their positions refined using SHARP (LaFortelle et al., *Methods in Enzymology*, 276, (1997), 472-494 and LaFortelle et al., Maximum Likelihood Refinement in a Graphical environment, with SHARP, in *CCP4 study week-end: Recent Advances in Phasing*, ed. Wilson et al., Daresbury Laboratory, UK). The final model contained 19 selenium sites which were used to provide initial phasing. Solvent flattening and phase extension techniques were used to produce an interpretable electron density map.

The program O was used for model building. The experimental, solvent flattened electron density map was readily interpretable and secondary structural elements were clearly defined in the electron density bones (calculated with MAPMAN, see Kleywegt et al., *Acta Crystallographica*, D52, (1996b), 826-828). The main chain of one monomer could be traced nearly continuously, using the secondary structure template building functionality in O, and the selenium atoms identified using SHARP providing guidance for chain-tracing.

-26-

The complete main chain model of monomer A was manually rotated to correspond with the bones of the second monomer (B). Since the relative orientation of the two domains was slightly different in monomer B, it was optimised by rigid body refinement (using REFMAC, see Murshudov et al., *Acta Crystallographica*, D53, (1997), 24-255), keeping separate the two domains (residues 1-176 and 177-283).

The model was improved by three iterated cycles of restrained and individual isotropic maximum likelihood refinement with REFMAC (40-1.7D resolution) together with manual rebuilding in O. σ_A -weighted $2F_{\text{obs}} - F_{\text{calc}}$ and $F_{\text{obs}} - F_{\text{calc}}$ maps were used (Read, *Acta Crystallographica*, A42, (1986), 140-149), the former frequently informative even when contoured at only 0.8-0.9 map standard deviations. For difficult parts of the model, maps and models resulting from simulated annealing in CNS (Brunger et al., *Acta Crystallographica*, D54, (1998), 905-921) were also considered. Ordered water molecules were modelled by automated cycles of water addition and removal by ARP (Perrakis et al., *Acta Crystallographica*, D55, (1999), 1765-1770) and refinement by REFMAC, with a final cycle of refinement with bulk solvent correction using CNS to ensure good geometry.

The final model consists of 4290 non-hydrogen protein atoms, and 384 water molecules. All residues were modelled, but electron density was poor for C-terminal residues (A283, B282-3), as well as residues B187-193; the B-factors of these residues are high, approaching 80\AA^2 . Residues A251-259, B63-68 and B251-259, though visible, are also not well ordered and have B-factors approaching 60\AA^2 . Two residues (A4 and A273) have alternative conformations, and 12 surface-exposed side chains are disordered and were modelled as the most common rotamer at zero occupancy.

-27-

Table 3 provides model parameters and refinement statistics for a version of the model which is essentially the same as that of Table 1 but contains more water molecules and also two ethanediol molecules and a Tris molecule. Residues B188-192 of this version of the model were reconstructed using BUSTER (Bricogne, *Methods in Enzymology*, 276, (1997), 361-423) in its implementation with TNT (Tronrud, *Methods in Enzymology*, 277, (1997), 306-319) instead of by the symmetry operation described above under "PS Structural Characterization". The program DDQ (van den Akker et al., *Acta Crystallographica*, D55, (1999), 206-218) was used to assess local and global accuracy and satisfactory completion of refinement, by considering difference density peaks arising from the final model. σ_A -weighted difference maps were calculated in REFMAC, excluding water molecules from the model. Quality of the model and its geometry were assessed by OOPS (Kleywegt et al., OOPS-a-daisy, *CCP4/ESF-EACBM Newsletter on Protein Crystallography*, 30, (1994), 20-24), PROCHECK (Laskowski et al., *J. Applied Crystallography*, 26, (1993), 283-291) and WHATCHECK (Hooft et al., *Nature*, 381, (1996), 272). No serious deviations from expected values are present, and warnings either correspond to well-defined justifiable features or else poorly-visible features that have high B-factors anyway. There are no Ramachandran outliers, and 92.2% of residues lie in most favoured regions of the plot.

Identification of Likely Active Sites

Having solved the PS crystal structure it is now evident that in terms of their C_α coordinates, the ATP-binding domains of (i) class I amino-acid tRNA synthetases (tRS) (i.e. EtRS from *Thermus thermophilus*, Nureki et al., *Science*, 267, (1995) 1958-1965; QtRS from *E. coli*, Perona et al., *Biochemistry*, 32,

-28-

(1993) 8758-8771; MtRS from *Thermus aquaticus*, Mechulam et al., *J. of Molecular Biology*, 294, (1999), 1287-1297; and YtRS from *Bacillus stearothermophilus*, Brick et al., *J. of Molecular Biology*, 208, (1989), 83-98), (ii)

- 5 phosphopantetheine adenylyltransferase (PPAT) from *E. coli* (Izard et al., *EMBO Journal*, 18, (1999), 2021-2030) and (iii) CTP:glycerol-3-phosphate cytidylyltransferase (CGT) from *B. subtilis* (Weber et al., *Structure with Folding and Design*, 7, (1999), 1113-1124) are structurally similar to domain N of PS.

10

More specifically, the particular class of Rossman fold which characterises tRS, CGT and PPAT consists of five β -strands in a central sheet and a cleft between β -strands β 1 and β 4 at the adenosine-binding site (see Fig. 2c). PS also has these

15 features. In addition, in all four cases strand β 5 is followed by catalytically important residues which form the KMSKS motif discussed below), and for both PS and tRS strand β 5 leads directly into the next domain.

- 20 Furthermore, two sequence motifs, HIGH and KMSKS (Barker et al., *FEBS Letters*, 145, (1982), 191-193), are conserved in tRS proteins and also in the wider superfamily. From mutational studies (First et al., in *Biochemistry*, 32, (1993), 13644-13663) these motifs are known to be involved in ATP binding:
- 25 the HIGH motif binds the adenine portion of ATP (cytidine in CGT) and the KMSKS motif stabilises the β - and γ -phosphate groups. These motifs are also found in PS and correspond respectively to residues 34-37 and 185-189.

- 30 The location of the bound ATP adenine in the structure of QtRS corresponds to within 2 to 3D of the positions of the bound nucleotides in YtRS, PPAT and CGT, i.e. in the cleft between strands β 1 and β 4 of the Rossman fold and against the top of helix α 1 (the location of the HIGH motif). When this domain

-29-

of QtRS is aligned with domain N of PS the HIGH (actually HDGH in PS) residues line up very well and the QtRS-bound ATP fits nearly perfectly into the same cleft in PS. Despite this excellent match, there is a difference in the positions of the helices ϵ_{107} (in PS) and αI (in QtRS) relative to the Rossman domain. This is the location of the KMSKS motif. However, by changing conservatively the ϕ/n -angles of residues Val175, Pro176, Ile177 and Met178 which form the PS inter-domain linker main chain, domain C can be rotated sufficiently to align the KMSKS residues with their QtRS counterparts and thus involve them in phosphate binding.

Fig. 4 shows a Connolly surface generated around the proposed PS active sites. The skilled person would immediately recognise that residues shown in the figure would be involved in respective interactions with Mg^{2+} , ATP, pantoate and β -alanine.

The Connolly surface opens besides the ATP ribose group and the walls are formed by fully conserved residues, which are largely hydrophobic but include some polar groups. The catalytically essential Mg^{2+} ion is shown at its most likely position where it is bound to OG_{Ser188} , OH_{Tyr71} , $O^{\beta 1}_{ATP}$ and $O^{\gamma 1}_{ATP}$. This is also the proposed Mg^{2+} binding position in PPAT.

Slightly more speculatively, the most favourable conformer of pantoate is shown positioned in a cavity where it appears to satisfy the hydrophobic and hydrogen-bonding interactions of the substrate, as well as being suitably positioned for attack on ATP.

Binding positions for β -alanine may also be proposed, but with less certainty than the binding positions of ATP and pantoate. For example, the β -alanine carboxylate may bind in a conserved, positively charged pocket to Arg123, with Met30,

-30-

Phe62 and Tyr71 providing a hydrophobic patch to accommodate the two β -alanine methylene groups, and His126 being suitably positioned to deprotonate the NH_3^+ group.

- 5 A list of the residues which line the binding pockets is provided in Table 4. Some or all of these residues may be used to model PS active sites in the various aspects of the invention discussed above.

10 *Structure-Based Drug Design*

- Determination of the 3D structure of PS provides important information about the likely active sites of PS, particularly when comparisons are made with similar enzymes. This
15 information may then be used for rational design of PS inhibitors, e.g. by computational techniques which identify possible binding ligands for the active sites, by enabling linked-fragment approaches to drug design, and by enabling the identification and location of bound ligands using X-ray
20 crystallographic analysis. These techniques are discussed in more detail below.

- Greer et al. mentioned above describes an iterative approach to ligand design based on repeated sequences of computer
25 modelling, protein-ligand complex formation and X-ray analysis. Thus novel thymidylate synthase inhibitor series were designed *de novo* by Greer et al., and PS inhibitors may also be designed in the this way. More specifically, using e.g. GRID on the solved 3D structure of PS, a ligand (e.g. a
30 potential inhibitor) for PS may be designed that complements the functionalities of the PS active site(s). The ligand can then be synthesised, formed into a complex with PS, and the complex then analysed by X-ray crystallography to identify the actual position of the bound ligand. The structure and/or

-31-

functional groups of the ligand can then be adjusted, if necessary, in view of the results of the X-ray analysis, and the synthesis and analysis sequence repeated until an optimised ligand is obtained. Related approaches to structure-based drug design are also discussed in Bohacek et al., *Medicinal Research Reviews*, Vol.16, (1996), 3-50.

As a result of the determination of the PS 3D structure, more purely computational techniques for rational drug design may also be used to design PS inhibitors (for an overview of these techniques see e.g. Walters et al. mentioned above). For example, automated ligand-receptor docking programs (discussed e.g. by Jones et al. in *Current Opinion in Biotechnology*, Vol.6, (1995), 652-656) which require accurate information on the atomic coordinates of target receptors may be used to design potential PS inhibitors.

Linked-fragment approaches to drug design also require accurate information on the atomic coordinates of target receptors. The basic idea behind these approaches is to determine (computationally or experimentally) the binding locations of plural ligands to a target molecule, and then construct a molecular scaffold to connect the ligands together in such a way that their relative binding positions are preserved. The ligands may be provided computationally and modelled in a computer system, or provided in an experimental setting, wherein crystals according to the invention are provided and a plurality of ligands soaked separately or in mixed pools into the crystal prior to X-ray analysis and determination of their location.

The binding site of two or more ligands are determined and may be connected to form a potential lead compound that can be further refined using e.g. the iterative technique of Greer et

-32-

al. For a virtual linked-fragment approach see Verlinde et al., *J. of Computer-Aided Molecular Design*, 6, (1992), 131-147, and for NMR and X-ray approaches see Shuker et al., *Science*, 274, (1996), 1531-1534 and Stout et al., *Structure*, 6, (1998), 839-848. The use of these approaches to design PS inhibitors is made possible by the determination of the PS structure.

Many of the techniques and approaches to structure-based drug design described above rely at some stage on X-ray analysis to identify the binding position of a ligand in a ligand-protein complex. A common way of doing this is to perform X-ray crystallography on the complex, produce a difference Fourier electron density map, and associate a particular pattern of electron density with the ligand. However, in order to produce the map (as explained e.g. by Blundell et al. mentioned above) it is necessary to know beforehand the protein 3D structure (or at least the protein structure factors). Therefore, determination of the PS structure also allows difference Fourier electron density maps of PS-ligand complexes to be produced, which can greatly assist the process of rational drug design.

The approaches to structure-based drug design described above all require initial identification of possible compounds for interaction with target bio-molecule (in this case PS). Sometimes these compounds are known e.g. from the research literature. However, when they are not, or when novel compounds are wanted, a first stage of the drug design program may involve computer-based *in silico* screening of compound databases (such as the Cambridge Structural Database) with the aim of identifying compounds which interact with the active site or sites of the target bio-molecule. Screening selection criteria may be based on pharmacokinetic properties such as

-33-

metabolic stability and toxicity. However, determination of the PS structure allows the architecture and chemical nature of each PS active site to be identified, which in turn allows the geometric and functional constraints of a descriptor for the potential modulator of PS activity to be derived. The descriptor is, therefore, a type of virtual 3-D pharmacophore, which can also be used as selection criteria or filter for database screening.

Compounds which have a chemical structure selected using the methods of the invention described herein, wherein said compounds are PS modulators, form a further aspect of the invention. Such compounds may be used in methods of medical treatments, such as in the treatment of bacterial infections in the human or animal body. The compounds may be used alone or in conjunction with other anti-bacterial compounds to enhance their effect.

While the invention has been described in conjunction with the exemplary embodiments described above, many equivalent modifications and variations will be apparent to those skilled in the art when given this disclosure. Accordingly, the exemplary embodiments of the invention set forth are considered to be illustrative and not limiting. Various changes to the described embodiments may be made without departing from the spirit and scope of the invention.

-34-

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-36-

Table 1

REMARK Written by O version 6.2.1

REMARK Sun Dec 19 17:28:32 1999

5 CRYST1 66.031 78.075 77.126 90.00 103.71 90.00
 ORIGX1 1.000000 0.000000 0.000000 0.000000
 ORIGX2 0.000000 1.000000 0.000000 0.000000
 ORIGX3 0.000000 0.000000 1.000000 0.000000
 10 SCALE1 0.015144 0.000000 0.003694 0.000000
 SCALE2 0.000000 0.012808 0.000000 0.000000
 SCALE3 0.000000 0.000000 0.013346 0.000000

15 Monomer A

| | Atom type | X | Y | Z | Occ. | B | Atomic No. |
|----|---------------------|--------|--------|--------|------|-------|---------------|
| 20 | ATOM 1 N MET A 1 | 21.480 | 5.652 | 9.350 | 1.00 | 40.77 | 7 |
| | ATOM 2 CA MET A 1 | 22.828 | 6.214 | 9.115 | 1.00 | 37.51 | 6 |
| | ATOM 3 C MET A 1 | 23.471 | 6.721 | 10.394 | 1.00 | 37.12 | 6 |
| | ATOM 4 O MET A 1 | 22.954 | 7.659 | 10.999 | 1.00 | 37.52 | 8 |
| | ATOM 5 CB MET A 1 | 22.777 | 7.385 | 8.130 | 1.00 | 35.78 | 6 |
| 25 | ATOM 6 CG MET A 1 | 24.222 | 7.748 | 7.741 | 1.00 | 33.60 | 6 |
| | ATOM 7 SD MET A 1 | 24.158 | 8.882 | 6.335 | 1.00 | 30.36 | 16 |
| | ATOM 8 CE MET A 1 | 23.874 | 10.429 | 7.197 | 1.00 | 27.91 | 6 |
| | ATOM 9 N LEU A 2 | 24.565 | 6.125 | 10.835 | 1.00 | 33.76 | 7 |
| | ATOM 10 CA LEU A 2 | 25.238 | 6.573 | 12.014 | 1.00 | 33.24 | 6 |
| 30 | ATOM 11 C LEU A 2 | 26.150 | 7.745 | 11.696 | 1.00 | 32.31 | 6 |
| | ATOM 12 O LEU A 2 | 26.856 | 7.637 | 10.679 | 1.00 | 31.54 | 8 |
| | ATOM 13 CB LEU A 2 | 26.138 | 5.467 | 12.571 | 1.00 | 36.11 | 6 |
| | ATOM 14 CG LEU A 2 | 25.578 | 4.098 | 12.886 | 1.00 | 40.23 | 6 |
| | ATOM 15 CD1 LEU A 2 | 26.741 | 3.164 | 13.253 | 1.00 | 39.01 | 6 |
| 35 | ATOM 16 CD2 LEU A 2 | 24.566 | 4.121 | 14.018 | 1.00 | 40.87 | 6 |
| | ATOM 17 N ILE A 3 | 26.233 | 8.778 | 12.481 | 1.00 | 30.54 | 7 |
| | ATOM 18 CA ILE A 3 | 27.148 | 9.869 | 12.303 | 1.00 | 30.81 | 6 |
| | ATOM 19 C ILE A 3 | 28.090 | 9.801 | 13.509 | 1.00 | 31.50 | 6 |
| | ATOM 20 O ILE A 3 | 27.616 | 9.918 | 14.642 | 1.00 | 31.89 | 8 |
| 40 | ATOM 21 CB ILE A 3 | 26.523 | 11.280 | 12.249 | 1.00 | 31.52 | 6 |
| | ATOM 22 CG1 ILE A 3 | 25.579 | 11.383 | 11.041 | 1.00 | 34.35 | 6 |
| | ATOM 23 CG2 ILE A 3 | 27.610 | 12.348 | 12.227 | 1.00 | 33.27 | 6 |
| | ATOM 24 CD1 ILE A 3 | 24.913 | 12.769 | 11.018 | 1.00 | 34.98 | 6 |
| | ATOM 25 N ILE A 4 | 29.350 | 9.493 | 13.296 | 1.00 | 26.66 | 7 |
| 45 | ATOM 26 CA ILE A 4 | 30.352 | 9.345 | 14.340 | 1.00 | 27.86 | 6 |
| | ATOM 27 C ILE A 4 | 31.314 | 10.510 | 14.337 | 1.00 | 28.36 | 6 |
| | ATOM 28 O ILE A 4 | 31.896 | 10.956 | 13.322 | 1.00 | 26.38 | 8 |
| | ATOM 29 CB ILE A 4 | 31.105 | 7.998 | 14.143 | 1.00 | 27.57 | 6 |
| | ATOM 30 CG1 ILE A 4 | 30.125 | 6.847 | 13.972 | 0.50 | 27.40 | 6 |
| 50 | ATOM 31 CG2 ILE A 4 | 32.067 | 7.779 | 15.312 | 0.50 | 26.53 | 6 |
| | ATOM 32 CD1 ILE A 4 | 29.201 | 6.526 | 15.113 | 0.50 | 28.00 | 6 |
| | ATOM 33 N GLU A 5 | 31.633 | 11.053 | 15.537 | 1.00 | 25.12 | 7 |
| | ATOM 34 CA GLU A 5 | 32.526 | 12.186 | 15.655 | 1.00 | 28.91 | 6 |
| | ATOM 35 C GLU A 5 | 33.843 | 11.934 | 16.357 | 1.00 | 26.18 | 6 |
| 55 | ATOM 36 O GLU A 5 | 34.724 | 12.779 | 16.300 | 1.00 | 27.45 | 8 |
| | ATOM 37 CB GLU A 5 | 31.769 | 13.303 | 16.441 | 1.00 | 31.10 | 6 |
| | ATOM 38 CG GLU A 5 | 30.611 | 13.871 | 15.627 | 1.00 | 34.62 | 6 |
| | ATOM 39 CD GLU A 5 | 29.795 | 14.929 | 16.355 | 1.00 | 40.38 | 6 |
| | ATOM 40 OE1 GLU A 5 | 30.263 | 15.579 | 17.306 | 1.00 | 41.78 | 8 |
| 60 | ATOM 41 OE2 GLU A 5 | 28.625 | 15.153 | 15.971 | 1.00 | 43.11 | 8 |
| | ATOM 42 N THR A 6 | 33.976 | 10.823 | 17.094 | 1.00 | 27.41 | 7 |
| | ATOM 43 CA THR A 6 | 35.188 | 10.587 | 17.848 | 1.00 | 27.21 | 6 |
| | ATOM 44 C THR A 6 | 35.969 | 9.345 | 17.384 | 1.00 | 26.94 | 6 |
| | ATOM 45 O THR A 6 | 35.294 | 8.397 | 16.960 | 1.00 | 25.74 | 8 |
| 65 | ATOM 46 CB THR A 6 | 34.867 | 10.400 | 19.351 | 1.00 | 29.81 | 6 |
| | ATOM 47 OG1 THR A 6 | 34.175 | 9.170 | 19.608 | 1.00 | 30.13 | 8 |
| | ATOM 48 CG2 THR A 6 | 33.967 | 11.528 | 19.852 | 1.00 | 29.59 | 6 |
| | ATOM 49 N LEU A 7 | 37.249 | 9.359 | 17.679 | 1.00 | 27.76 | 7 |
| | ATOM 50 CA LEU A 7 | 38.052 | 8.175 | 17.280 | 1.00 | 27.99 | 6 |
| 70 | ATOM 51 C LEU A 7 | 37.684 | 6.899 | 18.006 | 1.00 | 29.61 | 6 |
| | ATOM 52 O LEU A 7 | 37.546 | 5.845 | 17.381 | 1.00 | 26.94 | 8 |
| | ATOM 53 CB LEU A 7 | 39.526 | 8.515 | 17.460 | 1.00 | 28.02 | 6 |
| | ATOM 54 CG LEU A 7 | 40.011 | 9.725 | 16.678 | 1.00 | 31.71 | 6 |

-37-

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 55 | CD1 | LEU | A | 7 | 41.523 | 9.840 | 16.799 | 1.00 | 34.04 | 6 |
| | ATOM | 56 | CD2 | LEU | A | 7 | 39.612 | 9.641 | 15.219 | 1.00 | 32.76 | 6 |
| | ATOM | 57 | N | PRO | A | 8 | 37.434 | 6.913 | 19.313 | 1.00 | 30.58 | 7 |
| 5 | ATOM | 58 | CA | PRO | A | 8 | 37.081 | 5.687 | 20.013 | 1.00 | 29.86 | 6 |
| | ATOM | 59 | C | PRO | A | 8 | 35.814 | 5.062 | 19.505 | 1.00 | 28.23 | 6 |
| | ATOM | 60 | O | PRO | A | 8 | 35.701 | 3.845 | 19.394 | 1.00 | 25.90 | 8 |
| | ATOM | 61 | CB | PRO | A | 8 | 37.001 | 6.107 | 21.485 | 1.00 | 31.83 | 6 |
| | ATOM | 62 | CG | PRO | A | 8 | 37.816 | 7.345 | 21.593 | 1.00 | 31.44 | 6 |
| 10 | ATOM | 63 | CD | PRO | A | 8 | 37.601 | 8.053 | 20.243 | 1.00 | 30.62 | 6 |
| | ATOM | 64 | N | LEU | A | 9 | 34.754 | 5.838 | 19.239 | 1.00 | 27.49 | 7 |
| | ATOM | 65 | CA | LEU | A | 9 | 33.489 | 5.349 | 18.746 | 1.00 | 28.03 | 6 |
| | ATOM | 66 | C | LEU | A | 9 | 33.625 | 4.896 | 17.281 | 1.00 | 25.69 | 6 |
| | ATOM | 67 | O | LEU | A | 9 | 32.960 | 3.907 | 16.978 | 1.00 | 26.00 | 8 |
| 15 | ATOM | 68 | CB | LEU | A | 9 | 32.376 | 6.393 | 18.920 | 1.00 | 31.67 | 6 |
| | ATOM | 69 | CG | LEU | A | 9 | 32.089 | 6.741 | 20.400 | 1.00 | 35.64 | 6 |
| | ATOM | 70 | CD1 | LEU | A | 9 | 31.037 | 7.824 | 20.573 | 1.00 | 35.73 | 6 |
| | ATOM | 71 | CD2 | LEU | A | 9 | 31.636 | 5.493 | 21.154 | 1.00 | 37.26 | 6 |
| | ATOM | 72 | N | LEU | A | 10 | 34.532 | 5.512 | 16.526 | 1.00 | 25.45 | 7 |
| 20 | ATOM | 73 | CA | LEU | A | 10 | 34.763 | 5.045 | 15.154 | 1.00 | 23.19 | 6 |
| | ATOM | 74 | C | LEU | A | 10 | 35.461 | 3.678 | 15.228 | 1.00 | 23.87 | 6 |
| | ATOM | 75 | O | LEU | A | 10 | 35.017 | 2.730 | 14.592 | 1.00 | 23.85 | 8 |
| | ATOM | 76 | CB | LEU | A | 10 | 35.577 | 6.082 | 14.350 | 1.00 | 21.87 | 6 |
| | ATOM | 77 | CG | LEU | A | 10 | 36.012 | 5.560 | 12.953 | 1.00 | 22.51 | 6 |
| 25 | ATOM | 78 | CD1 | LEU | A | 10 | 34.829 | 5.397 | 12.007 | 1.00 | 22.75 | 6 |
| | ATOM | 79 | CD2 | LEU | A | 10 | 37.072 | 6.488 | 12.337 | 1.00 | 23.02 | 6 |
| | ATOM | 80 | N | ARG | A | 11 | 36.423 | 3.571 | 16.150 | 1.00 | 25.14 | 7 |
| | ATOM | 81 | CA | ARG | A | 11 | 37.191 | 2.304 | 16.232 | 1.00 | 28.37 | 6 |
| | ATOM | 82 | C | ARG | A | 11 | 36.236 | 1.209 | 16.642 | 1.00 | 29.20 | 6 |
| 30 | ATOM | 83 | O | ARG | A | 11 | 36.288 | 0.113 | 16.066 | 1.00 | 27.74 | 8 |
| | ATOM | 84 | CB | ARG | A | 11 | 38.399 | 2.556 | 17.142 | 1.00 | 31.48 | 6 |
| | ATOM | 85 | CG | ARG | A | 11 | 39.141 | 1.279 | 17.544 | 1.00 | 36.42 | 6 |
| | ATOM | 86 | CD | ARG | A | 11 | 40.384 | 1.586 | 18.401 | 1.00 | 40.76 | 6 |
| | ATOM | 87 | NE | ARG | A | 11 | 40.948 | 0.327 | 18.857 | 1.00 | 44.29 | 7 |
| 35 | ATOM | 88 | CZ | ARG | A | 11 | 40.627 | -0.524 | 19.819 | 1.00 | 45.48 | 6 |
| | ATOM | 89 | NH1 | ARG | A | 11 | 39.610 | -0.297 | 20.644 | 1.00 | 47.34 | 7 |
| | ATOM | 90 | NH2 | ARG | A | 11 | 41.306 | -1.656 | 20.008 | 1.00 | 45.04 | 7 |
| | ATOM | 91 | N | GLN | A | 12 | 35.347 | 1.474 | 17.591 | 1.00 | 26.32 | 7 |
| | ATOM | 92 | CA | GLN | A | 12 | 34.364 | 0.453 | 17.968 | 1.00 | 28.52 | 6 |
| 40 | ATOM | 93 | C | GLN | A | 12 | 33.550 | -0.050 | 16.798 | 1.00 | 27.48 | 6 |
| | ATOM | 94 | O | GLN | A | 12 | 33.340 | -1.248 | 16.579 | 1.00 | 25.61 | 8 |
| | ATOM | 95 | CB | GLN | A | 12 | 33.450 | 1.032 | 19.051 | 1.00 | 30.81 | 6 |
| | ATOM | 96 | CG | GLN | A | 12 | 32.364 | 0.022 | 19.483 | 1.00 | 34.43 | 6 |
| | ATOM | 97 | CD | GLN | A | 12 | 31.513 | 0.662 | 20.570 | 1.00 | 37.80 | 6 |
| 45 | ATOM | 98 | OE1 | GLN | A | 12 | 31.804 | 0.354 | 21.743 | 1.00 | 43.75 | 8 |
| | ATOM | 99 | NE2 | GLN | A | 12 | 30.545 | 1.495 | 20.293 | 1.00 | 38.11 | 7 |
| | ATOM | 100 | N | GLN | A | 13 | 32.938 | 0.879 | 16.025 | 1.00 | 25.56 | 7 |
| | ATOM | 101 | CA | GLN | A | 13 | 32.110 | 0.497 | 14.901 | 1.00 | 24.82 | 6 |
| | ATOM | 102 | C | GLN | A | 13 | 32.889 | -0.235 | 13.804 | 1.00 | 23.46 | 6 |
| 50 | ATOM | 103 | O | GLN | A | 13 | 32.360 | -1.209 | 13.326 | 1.00 | 24.23 | 8 |
| | ATOM | 104 | CB | GLN | A | 13 | 31.427 | 1.706 | 14.213 | 1.00 | 28.90 | 6 |
| | ATOM | 105 | CG | GLN | A | 13 | 30.471 | 2.397 | 15.154 | 1.00 | 34.73 | 6 |
| | ATOM | 106 | CD | GLN | A | 13 | 29.201 | 1.611 | 15.405 | 1.00 | 37.69 | 6 |
| | ATOM | 107 | OE1 | GLN | A | 13 | 28.697 | 0.913 | 14.519 | 1.00 | 40.12 | 8 |
| 55 | ATOM | 108 | NE2 | GLN | A | 13 | 28.765 | 1.760 | 16.646 | 1.00 | 39.64 | 7 |
| | ATOM | 109 | N | ILE | A | 14 | 34.075 | 0.258 | 13.493 | 1.00 | 21.48 | 7 |
| | ATOM | 110 | CA | ILE | A | 14 | 34.904 | -0.413 | 12.482 | 1.00 | 23.36 | 6 |
| | ATOM | 111 | C | ILE | A | 14 | 35.252 | -1.833 | 12.978 | 1.00 | 23.78 | 6 |
| | ATOM | 112 | O | ILE | A | 14 | 35.100 | -2.754 | 12.163 | 1.00 | 24.98 | 8 |
| 60 | ATOM | 113 | CB | ILE | A | 14 | 36.157 | 0.388 | 12.154 | 1.00 | 24.05 | 6 |
| | ATOM | 114 | CG1 | ILE | A | 14 | 35.752 | 1.756 | 11.492 | 1.00 | 23.68 | 6 |
| | ATOM | 115 | CG2 | ILE | A | 14 | 37.152 | -0.372 | 11.258 | 1.00 | 23.44 | 6 |
| | ATOM | 116 | CD1 | ILE | A | 14 | 34.981 | 1.571 | 10.185 | 1.00 | 22.33 | 6 |
| | ATOM | 117 | N | ARG | A | 15 | 35.691 | -1.946 | 14.210 | 1.00 | 24.68 | 7 |
| 65 | ATOM | 118 | CA | ARG | A | 15 | 36.062 | -3.331 | 14.658 | 1.00 | 24.36 | 6 |
| | ATOM | 119 | C | ARG | A | 15 | 34.868 | -4.230 | 14.500 | 1.00 | 24.62 | 6 |
| | ATOM | 120 | O | ARG | A | 15 | 34.925 | -5.358 | 13.991 | 1.00 | 26.61 | 8 |
| | ATOM | 121 | CB | ARG | A | 15 | 36.618 | -3.304 | 16.087 | 1.00 | 24.77 | 6 |
| | ATOM | 122 | CG | ARG | A | 15 | 38.037 | -2.760 | 16.169 | 1.00 | 29.78 | 6 |
| 70 | ATOM | 123 | CD | ARG | A | 15 | 38.488 | -2.556 | 17.609 | 1.00 | 31.54 | 6 |
| | ATOM | 124 | NE | ARG | A | 15 | 38.632 | -3.872 | 18.241 | 1.00 | 34.58 | 7 |
| | ATOM | 125 | CZ | ARG | A | 15 | 39.603 | -4.741 | 17.996 | 1.00 | 36.36 | 6 |
| | ATOM | 126 | NH1 | ARG | A | 15 | 40.588 | -4.484 | 17.142 | 1.00 | 37.87 | 7 |
| | ATOM | 127 | NH2 | ARG | A | 15 | 39.609 | -5.896 | 18.638 | 1.00 | 37.41 | 7 |
| | ATOM | 128 | N | ARG | A | 16 | 33.681 | -3.788 | 14.925 | 1.00 | 23.16 | 7 |

-38-

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|----|--------|---------|--------|------|-------|----|
| | ATOM | 129 | CA | ARG | A | 16 | 32.495 | -4.643 | 14.843 | 1.00 | 24.97 | 6 |
| | ATOM | 130 | C | ARG | A | 16 | 32.091 | -5.007 | 13.453 | 1.00 | 26.58 | 6 |
| | ATOM | 131 | O | ARG | A | 16 | 31.688 | -6.112 | 13.134 | 1.00 | 25.54 | 8 |
| 5 | ATOM | 132 | CB | ARG | A | 16 | 31.335 | -3.905 | 15.565 | 1.00 | 26.81 | 6 |
| | ATOM | 133 | CG | ARG | A | 16 | 31.739 | -3.858 | 17.037 | 1.00 | 30.82 | 6 |
| | ATOM | 134 | CD | ARG | A | 16 | 30.609 | -3.393 | 17.953 | 1.00 | 35.27 | 6 |
| | ATOM | 135 | NE | ARG | A | 16 | 31.145 | -3.440 | 19.331 | 1.00 | 38.72 | 7 |
| | ATOM | 136 | CZ | ARG | A | 16 | 30.380 | -3.407 | 20.431 | 1.00 | 41.50 | 6 |
| 10 | ATOM | 137 | NH1 | ARG | A | 16 | 29.057 | -3.350 | 20.279 | 1.00 | 41.64 | 7 |
| | ATOM | 138 | NH2 | ARG | A | 16 | 30.986 | -3.478 | 21.616 | 1.00 | 40.81 | 7 |
| | ATOM | 139 | N | LEU | A | 17 | 32.236 | -4.016 | 12.503 | 1.00 | 25.60 | 7 |
| | ATOM | 140 | CA | LEU | A | 17 | 31.869 | -4.342 | 11.148 | 1.00 | 25.51 | 6 |
| | ATOM | 141 | C | LEU | A | 17 | 32.796 | -5.382 | 10.547 | 1.00 | 25.77 | 6 |
| 15 | ATOM | 142 | O | LEU | A | 17 | 32.287 | -6.296 | 9.882 | 1.00 | 27.72 | 8 |
| | ATOM | 143 | CB | LEU | A | 17 | 31.929 | -3.067 | 10.251 | 1.00 | 26.53 | 6 |
| | ATOM | 144 | CG | LEU | A | 17 | 30.763 | -2.131 | 10.574 | 1.00 | 28.03 | 6 |
| | ATOM | 145 | CD1 | LEU | A | 17 | 31.127 | -0.707 | 10.125 | 1.00 | 29.84 | 6 |
| | ATOM | 146 | CD2 | LEU | A | 17 | 29.455 | -2.554 | 9.941 | 1.00 | 30.48 | 6 |
| 20 | ATOM | 147 | N | ARG | A | 18 | 34.062 | -5.187 | 10.811 | 1.00 | 25.72 | 7 |
| | ATOM | 148 | CA | ARG | A | 18 | 35.021 | -6.172 | 10.278 | 1.00 | 26.50 | 6 |
| | ATOM | 149 | C | ARG | A | 18 | 34.894 | -7.544 | 10.989 | 1.00 | 27.79 | 6 |
| | ATOM | 150 | O | ARG | A | 18 | 34.993 | -8.564 | 10.329 | 1.00 | 26.32 | 8 |
| | ATOM | 151 | CB | ARG | A | 18 | 36.436 | -5.665 | 10.405 | 1.00 | 28.86 | 6 |
| 25 | ATOM | 152 | CG | ARG | A | 18 | 36.506 | -4.291 | 9.685 | 1.00 | 31.17 | 6 |
| | ATOM | 153 | CD | ARG | A | 18 | 37.972 | -4.010 | 9.471 | 1.00 | 36.04 | 6 |
| | ATOM | 154 | NE | ARG | A | 18 | 38.502 | -4.834 | 8.364 | 1.00 | 39.73 | 7 |
| | ATOM | 155 | CZ | ARG | A | 18 | 39.788 | -5.197 | 8.409 | 1.00 | 41.34 | 6 |
| | ATOM | 156 | NH1 | ARG | A | 18 | 40.523 | -4.806 | 9.456 | 1.00 | 42.67 | 7 |
| 30 | ATOM | 157 | NH2 | ARG | A | 18 | 40.324 | -5.921 | 7.432 | 1.00 | 41.84 | 7 |
| | ATOM | 158 | N | MET | A | 19 | 34.537 | -7.458 | 12.259 | 1.00 | 25.78 | 7 |
| | ATOM | 159 | CA | MET | A | 19 | 34.344 | -8.735 | 13.010 | 1.00 | 27.53 | 6 |
| | ATOM | 160 | C | MET | A | 19 | 33.230 | -9.524 | 12.371 | 1.00 | 26.64 | 6 |
| | ATOM | 161 | O | MET | A | 19 | 33.236 | -10.747 | 12.181 | 1.00 | 25.81 | 8 |
| 35 | ATOM | 162 | CB | MET | A | 19 | 34.097 | -8.377 | 14.473 | 1.00 | 24.76 | 6 |
| | ATOM | 163 | CG | MET | A | 19 | 33.680 | -9.547 | 15.350 | 1.00 | 26.07 | 6 |
| | ATOM | 164 | SD | MET | A | 19 | 31.960 | -10.075 | 15.286 | 1.00 | 24.59 | 16 |
| | ATOM | 165 | CE | MET | A | 19 | 31.123 | -8.581 | 15.796 | 1.00 | 28.15 | 6 |
| | ATOM | 166 | N | GLU | A | 20 | 32.202 | -8.844 | 11.855 | 1.00 | 28.38 | 7 |
| 40 | ATOM | 167 | CA | GLU | A | 20 | 31.083 | -9.471 | 11.156 | 1.00 | 28.35 | 6 |
| | ATOM | 168 | C | GLU | A | 20 | 31.345 | -9.875 | 9.720 | 1.00 | 31.76 | 6 |
| | ATOM | 169 | O | GLU | A | 20 | 30.395 | -10.362 | 9.077 | 1.00 | 32.53 | 8 |
| | ATOM | 170 | CB | GLU | A | 20 | 29.874 | -8.502 | 11.103 | 1.00 | 30.90 | 6 |
| | ATOM | 171 | CG | GLU | A | 20 | 29.474 | -8.103 | 12.493 | 1.00 | 31.14 | 6 |
| 45 | ATOM | 172 | N | GLY | A | 21 | 32.531 | -9.676 | 9.217 | 1.00 | 29.46 | 7 |
| | ATOM | 173 | CA | GLY | A | 21 | 32.968 | -10.045 | 7.901 | 1.00 | 30.44 | 6 |
| | ATOM | 174 | C | GLY | A | 21 | 32.503 | -9.016 | 6.844 | 1.00 | 28.10 | 6 |
| | ATOM | 175 | O | GLY | A | 21 | 32.465 | -9.457 | 5.705 | 1.00 | 30.38 | 8 |
| | ATOM | 176 | N | LYS | A | 22 | 32.195 | -7.815 | 7.269 | 1.00 | 27.01 | 7 |
| 50 | ATOM | 177 | CA | LYS | A | 22 | 31.684 | -6.909 | 6.184 | 1.00 | 26.80 | 6 |
| | ATOM | 178 | C | LYS | A | 22 | 32.855 | -6.293 | 5.441 | 1.00 | 26.41 | 6 |
| | ATOM | 179 | O | LYS | A | 22 | 33.844 | -5.944 | 6.097 | 1.00 | 27.41 | 8 |
| | ATOM | 180 | CB | LYS | A | 22 | 30.773 | -5.883 | 6.825 | 1.00 | 27.50 | 6 |
| | ATOM | 181 | CG | LYS | A | 22 | 29.392 | -6.529 | 7.152 | 1.00 | 32.21 | 6 |
| 55 | ATOM | 182 | CD | LYS | A | 22 | 28.721 | -5.570 | 8.118 | 1.00 | 37.87 | 6 |
| | ATOM | 183 | CE | LYS | A | 22 | 27.207 | -5.752 | 8.159 | 1.00 | 42.38 | 6 |
| | ATOM | 184 | NZ | LYS | A | 22 | 26.574 | -4.400 | 8.447 | 1.00 | 46.00 | 7 |
| | ATOM | 185 | N | ARG | A | 23 | 32.737 | -6.159 | 4.128 | 1.00 | 26.60 | 7 |
| | ATOM | 186 | CA | ARG | A | 23 | 33.781 | -5.503 | 3.325 | 1.00 | 27.62 | 6 |
| 60 | ATOM | 187 | C | ARG | A | 23 | 33.468 | -4.008 | 3.350 | 1.00 | 25.54 | 6 |
| | ATOM | 188 | O | ARG | A | 23 | 32.293 | -3.677 | 3.209 | 1.00 | 25.62 | 8 |
| | ATOM | 189 | CB | ARG | A | 23 | 33.784 | -6.101 | 1.934 | 1.00 | 31.46 | 6 |
| | ATOM | 190 | CG | ARG | A | 23 | 34.506 | -5.433 | 0.801 | 1.00 | 39.27 | 6 |
| | ATOM | 191 | CD | ARG | A | 23 | 34.206 | -5.965 | -0.610 | 1.00 | 43.15 | 6 |
| 65 | ATOM | 192 | NE | ARG | A | 23 | 35.366 | -5.731 | -1.466 | 1.00 | 45.63 | 7 |
| | ATOM | 193 | CZ | ARG | A | 23 | 36.577 | -6.268 | -1.262 | 1.00 | 46.18 | 6 |
| | ATOM | 194 | NH1 | ARG | A | 23 | 36.841 | -7.101 | -0.272 | 1.00 | 47.31 | 7 |
| | ATOM | 195 | NH2 | ARG | A | 23 | 37.537 | -5.954 | -2.117 | 1.00 | 48.28 | 7 |
| | ATOM | 196 | N | VAL | A | 24 | 34.412 | -3.165 | 3.697 | 1.00 | 23.62 | 7 |
| 70 | ATOM | 197 | CA | VAL | A | 24 | 34.196 | -1.743 | 3.900 | 1.00 | 22.06 | 6 |
| | ATOM | 198 | C | VAL | A | 24 | 34.785 | -0.891 | 2.782 | 1.00 | 17.49 | 6 |
| | ATOM | 199 | O | VAL | A | 24 | 35.924 | -1.166 | 2.392 | 1.00 | 18.13 | 8 |
| | ATOM | 200 | CB | VAL | A | 24 | 34.830 | -1.279 | 5.218 | 1.00 | 22.91 | 6 |
| | ATOM | 201 | CG1 | VAL | A | 24 | 34.677 | 0.198 | 5.452 | 1.00 | 24.86 | 6 |
| | ATOM | 202 | CG2 | VAL | A | 24 | 34.173 | -2.010 | 6.405 | 1.00 | 24.10 | 6 |

-39-

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|----|
| | ATOM | 203 | N | ALA | A | 25 | 34.023 | 0.099 | 2.315 | 1.00 | 17.82 | 7 |
| | ATOM | 204 | CA | ALA | A | 25 | 34.597 | 0.939 | 1.279 | 1.00 | 18.16 | 6 |
| | ATOM | 205 | C | ALA | A | 25 | 34.593 | 2.272 | 2.004 | 1.00 | 18.48 | 6 |
| 5 | ATOM | 206 | O | ALA | A | 25 | 33.673 | 2.667 | 2.768 | 1.00 | 22.08 | 8 |
| | ATOM | 207 | CB | ALA | A | 25 | 33.863 | 1.032 | -0.030 | 1.00 | 20.30 | 6 |
| | ATOM | 208 | N | LEU | A | 26 | 35.579 | 3.142 | 1.726 | 1.00 | 16.71 | 7 |
| | ATOM | 209 | CA | LEU | A | 26 | 35.791 | 4.438 | 2.266 | 1.00 | 16.65 | 6 |
| | ATOM | 210 | C | LEU | A | 26 | 35.819 | 5.507 | 1.152 | 1.00 | 17.57 | 6 |
| 10 | ATOM | 211 | O | LEU | A | 26 | 36.497 | 5.321 | 0.146 | 1.00 | 18.90 | 8 |
| | ATOM | 212 | CB | LEU | A | 26 | 37.120 | 4.628 | 3.038 | 1.00 | 18.22 | 6 |
| | ATOM | 213 | CG | LEU | A | 26 | 37.458 | 6.066 | 3.461 | 1.00 | 18.69 | 6 |
| | ATOM | 214 | CD1 | LEU | A | 26 | 36.500 | 6.657 | 4.511 | 1.00 | 20.43 | 6 |
| | ATOM | 215 | CD2 | LEU | A | 26 | 38.887 | 6.061 | 4.006 | 1.00 | 20.45 | 6 |
| 15 | ATOM | 216 | N | VAL | A | 27 | 35.065 | 6.569 | 1.318 | 1.00 | 16.54 | 7 |
| | ATOM | 217 | CA | VAL | A | 27 | 35.028 | 7.712 | 0.418 | 1.00 | 16.69 | 6 |
| | ATOM | 218 | C | VAL | A | 27 | 35.493 | 8.915 | 1.208 | 1.00 | 15.96 | 6 |
| | ATOM | 219 | O | VAL | A | 27 | 34.643 | 9.495 | 1.891 | 1.00 | 17.62 | 8 |
| | ATOM | 220 | CB | VAL | A | 27 | 33.636 | 8.038 | -0.196 | 1.00 | 18.00 | 6 |
| 20 | ATOM | 221 | CG1 | VAL | A | 27 | 33.738 | 9.238 | -1.157 | 1.00 | 21.63 | 6 |
| | ATOM | 222 | CG2 | VAL | A | 27 | 33.057 | 6.801 | -0.869 | 1.00 | 20.05 | 6 |
| | ATOM | 223 | N | PRO | A | 28 | 36.728 | 9.403 | 1.100 | 1.00 | 18.63 | 7 |
| | ATOM | 224 | CA | PRO | A | 28 | 37.265 | 10.543 | 1.776 | 1.00 | 19.42 | 6 |
| | ATOM | 225 | C | PRO | A | 28 | 36.814 | 11.864 | 1.198 | 1.00 | 20.36 | 6 |
| 25 | ATOM | 226 | O | PRO | A | 28 | 36.941 | 11.994 | -0.024 | 1.00 | 21.38 | 8 |
| | ATOM | 227 | CB | PRO | A | 28 | 38.775 | 10.466 | 1.589 | 1.00 | 23.04 | 6 |
| | ATOM | 228 | CG | PRO | A | 28 | 39.036 | 9.147 | 0.945 | 1.00 | 23.71 | 6 |
| | ATOM | 229 | CD | PRO | A | 28 | 37.765 | 8.641 | 0.309 | 1.00 | 19.69 | 6 |
| | ATOM | 230 | N | THR | A | 29 | 36.209 | 12.765 | 1.957 | 1.00 | 20.05 | 7 |
| 30 | ATOM | 231 | CA | THR | A | 29 | 35.752 | 14.046 | 1.426 | 1.00 | 20.41 | 6 |
| | ATOM | 232 | C | THR | A | 29 | 36.036 | 15.159 | 2.439 | 1.00 | 18.55 | 6 |
| | ATOM | 233 | O | THR | A | 29 | 36.271 | 14.922 | 3.618 | 1.00 | 19.34 | 8 |
| | ATOM | 234 | CB | THR | A | 29 | 34.254 | 14.069 | 1.053 | 1.00 | 21.16 | 6 |
| | ATOM | 235 | OG1 | THR | A | 29 | 33.512 | 14.439 | 2.242 | 1.00 | 19.82 | 8 |
| 35 | ATOM | 236 | CG2 | THR | A | 29 | 33.658 | 12.762 | 0.537 | 1.00 | 20.33 | 6 |
| | ATOM | 237 | N | MET | A | 30 | 35.897 | 16.391 | 2.003 | 1.00 | 20.47 | 7 |
| | ATOM | 238 | CA | MET | A | 30 | 35.998 | 17.616 | 2.811 | 1.00 | 20.82 | 6 |
| | ATOM | 239 | C | MET | A | 30 | 34.587 | 18.281 | 2.815 | 1.00 | 23.33 | 6 |
| | ATOM | 240 | O | MET | A | 30 | 34.465 | 19.488 | 3.115 | 1.00 | 23.42 | 8 |
| 40 | ATOM | 241 | CB | MET | A | 30 | 37.065 | 18.623 | 2.375 | 1.00 | 21.06 | 6 |
| | ATOM | 242 | CG | MET | A | 30 | 38.446 | 17.925 | 2.357 | 1.00 | 21.02 | 6 |
| | ATOM | 243 | SD | MET | A | 30 | 39.740 | 19.108 | 2.816 | 1.00 | 24.24 | 16 |
| | ATOM | 244 | CE | MET | A | 30 | 39.431 | 20.461 | 1.687 | 1.00 | 26.95 | 6 |
| | ATOM | 245 | N | GLY | A | 31 | 33.576 | 17.477 | 2.616 | 1.00 | 21.21 | 7 |
| 45 | ATOM | 246 | CA | GLY | A | 31 | 32.189 | 17.985 | 2.705 | 1.00 | 24.38 | 6 |
| | ATOM | 247 | C | GLY | A | 31 | 31.835 | 18.946 | 1.563 | 1.00 | 24.71 | 6 |
| | ATOM | 248 | O | GLY | A | 31 | 32.498 | 18.909 | 0.524 | 1.00 | 22.94 | 8 |
| | ATOM | 249 | N | ASN | A | 32 | 30.712 | 19.650 | 1.637 | 1.00 | 24.08 | 7 |
| | ATOM | 250 | CA | ASN | A | 32 | 30.269 | 20.550 | 0.552 | 1.00 | 22.88 | 6 |
| 50 | ATOM | 251 | C | ASN | A | 32 | 29.995 | 19.636 | -0.655 | 1.00 | 22.70 | 6 |
| | ATOM | 252 | O | ASN | A | 32 | 30.519 | 19.801 | -1.762 | 1.00 | 25.35 | 8 |
| | ATOM | 253 | CB | ASN | A | 32 | 31.269 | 21.654 | 0.253 | 1.00 | 27.38 | 6 |
| | ATOM | 254 | CG | ASN | A | 32 | 30.612 | 22.708 | -0.658 | 1.00 | 31.01 | 6 |
| | ATOM | 255 | OD1 | ASN | A | 32 | 29.390 | 22.842 | -0.531 | 1.00 | 33.26 | 8 |
| 55 | ATOM | 256 | ND2 | ASN | A | 32 | 31.392 | 23.283 | -1.538 | 1.00 | 31.51 | 7 |
| | ATOM | 257 | N | LEU | A | 33 | 29.250 | 18.551 | -0.428 | 1.00 | 22.17 | 7 |
| | ATOM | 258 | CA | LEU | A | 33 | 29.111 | 17.438 | -1.343 | 1.00 | 20.92 | 6 |
| | ATOM | 259 | C | LEU | A | 33 | 28.300 | 17.796 | -2.594 | 1.00 | 23.49 | 6 |
| | ATOM | 260 | O | LEU | A | 33 | 27.325 | 18.519 | -2.397 | 1.00 | 25.06 | 8 |
| 60 | ATOM | 261 | CB | LEU | A | 33 | 28.479 | 16.200 | -0.668 | 1.00 | 21.06 | 6 |
| | ATOM | 262 | CG | LEU | A | 33 | 29.372 | 15.713 | 0.501 | 1.00 | 21.76 | 6 |
| | ATOM | 263 | CD1 | LEU | A | 33 | 28.821 | 14.431 | 1.108 | 1.00 | 24.92 | 6 |
| | ATOM | 264 | CD2 | LEU | A | 33 | 30.834 | 15.495 | 0.073 | 1.00 | 21.13 | 6 |
| | ATOM | 265 | N | HIS | A | 34 | 28.691 | 17.217 | -3.706 | 1.00 | 21.31 | 7 |
| 65 | ATOM | 266 | CA | HIS | A | 34 | 27.929 | 17.454 | -4.953 | 1.00 | 19.68 | 6 |
| | ATOM | 267 | C | HIS | A | 34 | 27.793 | 16.165 | -5.698 | 1.00 | 21.69 | 6 |
| | ATOM | 268 | O | HIS | A | 34 | 28.073 | 15.035 | -5.218 | 1.00 | 21.01 | 8 |
| | ATOM | 269 | CB | HIS | A | 34 | 28.648 | 18.575 | -5.722 | 1.00 | 20.00 | 6 |
| | ATOM | 270 | CG | HIS | A | 34 | 30.062 | 18.267 | -6.078 | 1.00 | 23.69 | 6 |
| 70 | ATOM | 271 | ND1 | HIS | A | 34 | 30.449 | 17.170 | -6.770 | 1.00 | 26.07 | 7 |
| | ATOM | 272 | CD2 | HIS | A | 34 | 31.211 | 18.953 | -5.778 | 1.00 | 26.19 | 6 |
| | ATOM | 273 | CE1 | HIS | A | 34 | 31.776 | 17.161 | -6.890 | 1.00 | 27.03 | 6 |
| | ATOM | 274 | NE2 | HIS | A | 34 | 32.262 | 18.221 | -6.296 | 1.00 | 27.65 | 7 |
| | ATOM | 275 | N | ASP | A | 35 | 27.277 | 16.218 | -6.957 | 1.00 | 20.96 | 7 |
| | ATOM | 276 | CA | ASP | A | 35 | 26.992 | 15.008 | -7.685 | 1.00 | 21.21 | 6 |

-40-

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|----|
| | ATOM | 277 | C | ASP | A | 35 | 28.213 | 14.132 | -7.962 | 1.00 | 20.16 | 6 |
| | ATOM | 278 | O | ASP | A | 35 | 28.006 | 12.921 | -8.079 | 1.00 | 22.17 | 8 |
| | ATOM | 279 | CB | ASP | A | 35 | 26.386 | 15.393 | -9.061 | 1.00 | 23.09 | 6 |
| 5 | ATOM | 280 | CG | ASP | A | 35 | 24.959 | 15.842 | -8.957 | 1.00 | 26.28 | 6 |
| | ATOM | 281 | OD1 | ASP | A | 35 | 24.273 | 15.662 | -7.929 | 1.00 | 27.10 | 8 |
| | ATOM | 282 | OD2 | ASP | A | 35 | 24.439 | 16.326 | -10.018 | 1.00 | 25.60 | 8 |
| | ATOM | 283 | N | GLY | A | 36 | 29.375 | 14.766 | -8.056 | 1.00 | 21.98 | 7 |
| | ATOM | 284 | CA | GLY | A | 36 | 30.620 | 14.030 | -8.244 | 1.00 | 21.77 | 6 |
| 10 | ATOM | 285 | C | GLY | A | 36 | 30.786 | 13.041 | -7.065 | 1.00 | 22.77 | 6 |
| | ATOM | 286 | O | GLY | A | 36 | 31.157 | 11.870 | -7.245 | 1.00 | 22.33 | 8 |
| | ATOM | 287 | N | HIS | A | 37 | 30.620 | 13.573 | -5.849 | 1.00 | 22.48 | 7 |
| | ATOM | 288 | CA | HIS | A | 37 | 30.753 | 12.759 | -4.642 | 1.00 | 19.90 | 6 |
| | ATOM | 289 | C | HIS | A | 37 | 29.688 | 11.715 | -4.564 | 1.00 | 20.48 | 6 |
| 15 | ATOM | 290 | O | HIS | A | 37 | 29.886 | 10.568 | -4.111 | 1.00 | 20.51 | 8 |
| | ATOM | 291 | CB | HIS | A | 37 | 30.659 | 13.645 | -3.371 | 1.00 | 20.77 | 6 |
| | ATOM | 292 | CG | HIS | A | 37 | 31.604 | 14.773 | -3.310 | 1.00 | 23.28 | 6 |
| | ATOM | 293 | ND1 | HIS | A | 37 | 32.947 | 14.667 | -2.929 | 1.00 | 28.53 | 7 |
| | ATOM | 294 | CD2 | HIS | A | 37 | 31.407 | 16.089 | -3.544 | 1.00 | 19.82 | 6 |
| 20 | ATOM | 295 | CE1 | HIS | A | 37 | 33.536 | 15.843 | -2.870 | 1.00 | 23.53 | 6 |
| | ATOM | 296 | NE2 | HIS | A | 37 | 32.585 | 16.736 | -3.250 | 1.00 | 26.84 | 7 |
| | ATOM | 297 | N | MET | A | 38 | 28.469 | 11.976 | -5.080 | 1.00 | 19.18 | 7 |
| | ATOM | 298 | CA | MET | A | 38 | 27.409 | 10.961 | -5.035 | 1.00 | 19.76 | 6 |
| | ATOM | 299 | C | MET | A | 38 | 27.795 | 9.798 | -5.955 | 1.00 | 22.39 | 6 |
| 25 | ATOM | 300 | O | MET | A | 38 | 27.476 | 8.670 | -5.614 | 1.00 | 21.94 | 8 |
| | ATOM | 301 | CB | MET | A | 38 | 26.038 | 11.520 | -5.422 | 1.00 | 23.14 | 6 |
| | ATOM | 302 | CG | MET | A | 38 | 25.482 | 12.594 | -4.447 | 1.00 | 25.87 | 6 |
| | ATOM | 303 | SD | MET | A | 38 | 25.332 | 11.996 | -2.726 | 1.00 | 28.93 | 16 |
| | ATOM | 304 | CE | MET | A | 38 | 26.690 | 12.846 | -1.980 | 1.00 | 25.74 | 6 |
| 30 | ATOM | 305 | N | LYS | A | 39 | 28.493 | 10.034 | -7.069 | 1.00 | 19.54 | 7 |
| | ATOM | 306 | CA | LYS | A | 39 | 28.943 | 8.945 | -7.921 | 1.00 | 21.23 | 6 |
| | ATOM | 307 | C | LYS | A | 39 | 29.995 | 8.090 | -7.205 | 1.00 | 19.48 | 6 |
| | ATOM | 308 | O | LYS | A | 39 | 29.947 | 6.878 | -7.283 | 1.00 | 19.63 | 8 |
| | ATOM | 309 | CB | LYS | A | 39 | 29.524 | 9.474 | -9.236 | 1.00 | 23.04 | 6 |
| 35 | ATOM | 310 | CG | LYS | A | 39 | 29.977 | 8.354 | -10.200 | 1.00 | 23.73 | 6 |
| | ATOM | 311 | CD | LYS | A | 39 | 28.831 | 7.464 | -10.663 | 1.00 | 29.69 | 6 |
| | ATOM | 312 | CE | LYS | A | 39 | 29.392 | 6.340 | -11.576 | 1.00 | 32.23 | 6 |
| | ATOM | 313 | NZ | LYS | A | 39 | 28.207 | 5.549 | -12.095 | 1.00 | 35.95 | 7 |
| | ATOM | 314 | N | LEU | A | 40 | 30.869 | 8.716 | -6.387 | 1.00 | 18.59 | 7 |
| 40 | ATOM | 315 | CA | LEU | A | 40 | 31.829 | 7.935 | -5.587 | 1.00 | 19.30 | 6 |
| | ATOM | 316 | C | LEU | A | 40 | 31.065 | 7.001 | -4.652 | 1.00 | 17.32 | 6 |
| | ATOM | 317 | O | LEU | A | 40 | 31.433 | 5.818 | -4.467 | 1.00 | 19.58 | 8 |
| | ATOM | 318 | CB | LEU | A | 40 | 32.725 | 8.865 | -4.822 | 1.00 | 20.84 | 6 |
| | ATOM | 319 | CG | LEU | A | 40 | 33.577 | 9.868 | -5.641 | 1.00 | 21.98 | 6 |
| 45 | ATOM | 320 | CD1 | LEU | A | 40 | 34.510 | 10.649 | -4.714 | 1.00 | 19.78 | 6 |
| | ATOM | 321 | CD2 | LEU | A | 40 | 34.368 | 9.211 | -6.759 | 1.00 | 22.47 | 6 |
| | ATOM | 322 | N | VAL | A | 41 | 30.079 | 7.532 | -3.957 | 1.00 | 19.06 | 7 |
| | ATOM | 323 | CA | VAL | A | 41 | 29.260 | 6.732 | -3.016 | 1.00 | 18.09 | 6 |
| | ATOM | 324 | C | VAL | A | 41 | 28.598 | 5.614 | -3.736 | 1.00 | 17.62 | 6 |
| 50 | ATOM | 325 | O | VAL | A | 41 | 28.537 | 4.470 | -3.258 | 1.00 | 19.88 | 8 |
| | ATOM | 326 | CB | VAL | A | 41 | 28.253 | 7.674 | -2.265 | 1.00 | 20.51 | 6 |
| | ATOM | 327 | CG1 | VAL | A | 41 | 27.211 | 6.841 | -1.514 | 1.00 | 21.02 | 6 |
| | ATOM | 328 | CG2 | VAL | A | 41 | 29.010 | 8.629 | -1.336 | 1.00 | 19.99 | 6 |
| | ATOM | 329 | N | ASP | A | 42 | 28.010 | 5.882 | -4.952 | 1.00 | 18.32 | 7 |
| 55 | ATOM | 330 | CA | ASP | A | 42 | 27.355 | 4.768 | -5.614 | 1.00 | 20.18 | 6 |
| | ATOM | 331 | C | ASP | A | 42 | 28.312 | 3.653 | -5.995 | 1.00 | 20.77 | 6 |
| | ATOM | 332 | O | ASP | A | 42 | 27.977 | 2.483 | -5.943 | 1.00 | 22.32 | 8 |
| | ATOM | 333 | CB | ASP | A | 42 | 26.667 | 5.238 | -6.920 | 1.00 | 22.54 | 6 |
| | ATOM | 334 | CG | ASP | A | 42 | 25.531 | 6.164 | -6.652 | 1.00 | 24.06 | 6 |
| 60 | ATOM | 335 | OD1 | ASP | A | 42 | 24.908 | 6.188 | -5.570 | 1.00 | 27.49 | 8 |
| | ATOM | 336 | OD2 | ASP | A | 42 | 25.140 | 6.976 | -7.558 | 1.00 | 30.83 | 8 |
| | ATOM | 337 | N | GLU | A | 43 | 29.539 | 4.041 | -6.419 | 1.00 | 20.92 | 7 |
| | ATOM | 338 | CA | GLU | A | 43 | 30.528 | 3.015 | -6.753 | 1.00 | 22.39 | 6 |
| | ATOM | 339 | C | GLU | A | 43 | 30.924 | 2.224 | -5.512 | 1.00 | 21.74 | 6 |
| 65 | ATOM | 340 | O | GLU | A | 43 | 31.185 | 1.036 | -5.623 | 1.00 | 23.66 | 8 |
| | ATOM | 341 | CB | GLU | A | 43 | 31.816 | 3.583 | -7.342 | 1.00 | 23.36 | 6 |
| | ATOM | 342 | CG | GLU | A | 43 | 31.560 | 4.030 | -8.792 | 1.00 | 32.68 | 6 |
| | ATOM | 343 | CD | GLU | A | 43 | 31.450 | 2.806 | -9.705 | 1.00 | 34.94 | 6 |
| | ATOM | 344 | OE1 | GLU | A | 43 | 32.113 | 1.776 | -9.517 | 1.00 | 39.24 | 8 |
| 70 | ATOM | 345 | OE2 | GLU | A | 43 | 30.590 | 2.908 | -10.606 | 1.00 | 42.50 | 8 |
| | ATOM | 346 | N | ALA | A | 44 | 31.103 | 2.914 | -4.372 | 1.00 | 21.59 | 7 |
| | ATOM | 347 | CA | ALA | A | 44 | 31.413 | 2.228 | -3.131 | 1.00 | 20.24 | 6 |
| | ATOM | 348 | C | ALA | A | 44 | 30.241 | 1.299 | -2.736 | 1.00 | 22.05 | 6 |
| | ATOM | 349 | O | ALA | A | 44 | 30.575 | 0.162 | -2.324 | 1.00 | 23.77 | 8 |
| | ATOM | 350 | CB | ALA | A | 44 | 31.698 | 3.226 | -2.025 | 1.00 | 19.63 | 6 |

-41-

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|----|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|---|
| | ATOM | 351 | N | LYS | A | 45 | 29.033 | 1.800 | -2.843 | 1.00 | 24.11 | 7 |
| | ATOM | 352 | CA | LYS | A | 45 | 27.888 | 0.912 | -2.499 | 1.00 | 26.00 | 6 |
| | ATOM | 353 | C | LYS | A | 45 | 27.912 | -0.215 | -3.471 | 1.00 | 27.19 | 6 |
| 5 | ATOM | 354 | O | LYS | A | 45 | 27.573 | -1.297 | -2.970 | 1.00 | 28.01 | 8 |
| | ATOM | 355 | CB | LYS | A | 45 | 26.550 | 1.612 | -2.555 | 1.00 | 28.17 | 6 |
| | ATOM | 356 | CG | LYS | A | 45 | 26.331 | 2.723 | -1.544 | 1.00 | 33.53 | 6 |
| | ATOM | 357 | CD | LYS | A | 45 | 25.613 | 2.271 | -0.277 | 1.00 | 40.20 | 6 |
| | ATOM | 358 | CE | LYS | A | 45 | 24.365 | 1.437 | -0.586 | 1.00 | 42.16 | 6 |
| 10 | ATOM | 359 | NZ | LYS | A | 45 | 23.332 | 1.467 | 0.475 | 1.00 | 47.05 | 7 |
| | ATOM | 360 | N | ALA | A | 46 | 28.221 | -0.250 | -4.714 | 1.00 | 25.90 | 7 |
| | ATOM | 361 | CA | ALA | A | 46 | 28.227 | -1.457 | -5.529 | 1.00 | 26.79 | 6 |
| | ATOM | 362 | C | ALA | A | 46 | 29.360 | -2.424 | -5.183 | 1.00 | 29.75 | 6 |
| | ATOM | 363 | O | ALA | A | 46 | 29.233 | -3.661 | -5.395 | 1.00 | 28.75 | 8 |
| 15 | ATOM | 364 | CB | ALA | A | 46 | 28.360 | -1.038 | -6.984 | 1.00 | 28.50 | 6 |
| | ATOM | 365 | N | ARG | A | 47 | 30.492 | -1.922 | -4.680 | 1.00 | 26.27 | 7 |
| | ATOM | 366 | CA | ARG | A | 47 | 31.649 | -2.782 | -4.511 | 1.00 | 25.06 | 6 |
| | ATOM | 367 | C | ARG | A | 47 | 31.816 | -3.283 | -3.103 | 1.00 | 25.85 | 6 |
| | ATOM | 368 | O | ARG | A | 47 | 32.669 | -4.158 | -2.954 | 1.00 | 29.00 | 8 |
| 20 | ATOM | 369 | CB | ARG | A | 47 | 32.921 | -1.993 | -4.921 | 1.00 | 26.64 | 6 |
| | ATOM | 370 | CG | ARG | A | 47 | 32.973 | -1.664 | -6.407 | 1.00 | 30.45 | 6 |
| | ATOM | 371 | CD | ARG | A | 47 | 34.079 | -0.626 | -6.688 | 1.00 | 30.96 | 6 |
| | ATOM | 372 | NE | ARG | A | 47 | 33.831 | -0.063 | -8.068 | 1.00 | 36.09 | 7 |
| | ATOM | 373 | CZ | ARG | A | 47 | 34.612 | -0.526 | -9.051 | 1.00 | 37.23 | 6 |
| 25 | ATOM | 374 | NH1 | ARG | A | 47 | 35.552 | -1.422 | -8.779 | 1.00 | 37.53 | 7 |
| | ATOM | 375 | NH2 | ARG | A | 47 | 34.458 | -0.076 | -10.277 | 1.00 | 38.83 | 7 |
| | ATOM | 376 | N | ALA | A | 48 | 31.118 | -2.729 | -2.117 | 1.00 | 23.59 | 7 |
| | ATOM | 377 | CA | ALA | A | 48 | 31.382 | -3.211 | -0.762 | 1.00 | 23.32 | 6 |
| | ATOM | 378 | C | ALA | A | 48 | 30.099 | -3.421 | 0.008 | 1.00 | 23.85 | 6 |
| 30 | ATOM | 379 | O | ALA | A | 48 | 29.048 | -2.891 | -0.355 | 1.00 | 26.50 | 8 |
| | ATOM | 380 | CB | ALA | A | 48 | 32.316 | -2.196 | -0.069 | 1.00 | 24.37 | 6 |
| | ATOM | 381 | N | ASP | A | 49 | 30.163 | -4.115 | 1.146 | 1.00 | 22.20 | 7 |
| | ATOM | 382 | CA | ASP | A | 49 | 28.925 | -4.271 | 1.916 | 1.00 | 26.00 | 6 |
| | ATOM | 383 | C | ASP | A | 49 | 28.562 | -3.133 | 2.803 | 1.00 | 26.80 | 6 |
| 35 | ATOM | 384 | O | ASP | A | 49 | 27.400 | -2.841 | 3.120 | 1.00 | 28.51 | 8 |
| | ATOM | 385 | CB | ASP | A | 49 | 29.066 | -5.563 | 2.775 | 1.00 | 31.27 | 6 |
| | ATOM | 386 | CG | ASP | A | 49 | 29.809 | -6.700 | 2.149 | 1.00 | 35.17 | 6 |
| | ATOM | 387 | OD1 | ASP | A | 49 | 30.741 | -7.285 | 2.759 | 1.00 | 35.30 | 8 |
| | ATOM | 388 | OD2 | ASP | A | 49 | 29.459 | -7.142 | 1.032 | 1.00 | 39.32 | 8 |
| 40 | ATOM | 389 | N | VAL | A | 50 | 29.551 | -2.305 | 3.185 | 1.00 | 21.71 | 7 |
| | ATOM | 390 | CA | VAL | A | 50 | 29.379 | -1.186 | 4.072 | 1.00 | 24.23 | 6 |
| | ATOM | 391 | C | VAL | A | 50 | 30.120 | 0.032 | 3.514 | 1.00 | 22.66 | 6 |
| | ATOM | 392 | O | VAL | A | 50 | 31.259 | -0.150 | 3.088 | 1.00 | 23.46 | 8 |
| | ATOM | 393 | CB | VAL | A | 50 | 29.980 | -1.492 | 5.460 | 1.00 | 28.04 | 6 |
| 45 | ATOM | 394 | CG1 | VAL | A | 50 | 29.862 | -0.274 | 6.353 | 1.00 | 30.12 | 6 |
| | ATOM | 395 | CG2 | VAL | A | 50 | 29.310 | -2.723 | 6.087 | 1.00 | 31.57 | 6 |
| | ATOM | 396 | N | VAL | A | 51 | 29.462 | 1.181 | 3.484 | 1.00 | 20.55 | 7 |
| | ATOM | 397 | CA | VAL | A | 51 | 30.124 | 2.367 | 2.940 | 1.00 | 18.63 | 6 |
| | ATOM | 398 | C | VAL | A | 51 | 30.317 | 3.377 | 4.038 | 1.00 | 19.83 | 6 |
| 50 | ATOM | 399 | O | VAL | A | 51 | 29.382 | 3.743 | 4.754 | 1.00 | 19.84 | 8 |
| | ATOM | 400 | CB | VAL | A | 51 | 29.292 | 3.029 | 1.830 | 1.00 | 21.12 | 6 |
| | ATOM | 401 | CG1 | VAL | A | 51 | 29.993 | 4.288 | 1.310 | 1.00 | 22.56 | 6 |
| | ATOM | 402 | CG2 | VAL | A | 51 | 29.015 | 2.098 | 0.666 | 1.00 | 23.68 | 6 |
| | ATOM | 403 | N | VAL | A | 52 | 31.527 | 3.878 | 4.198 | 1.00 | 18.34 | 7 |
| 55 | ATOM | 404 | CA | VAL | A | 52 | 31.884 | 4.890 | 5.151 | 1.00 | 18.76 | 6 |
| | ATOM | 405 | C | VAL | A | 52 | 32.298 | 6.183 | 4.450 | 1.00 | 20.80 | 6 |
| | ATOM | 406 | O | VAL | A | 52 | 33.147 | 6.104 | 3.559 | 1.00 | 21.14 | 8 |
| | ATOM | 407 | CB | VAL | A | 52 | 33.088 | 4.473 | 6.034 | 1.00 | 20.37 | 6 |
| | ATOM | 408 | CG1 | VAL | A | 52 | 33.539 | 5.585 | 6.978 | 1.00 | 19.87 | 6 |
| 60 | ATOM | 409 | CG2 | VAL | A | 52 | 32.719 | 3.217 | 6.820 | 1.00 | 21.14 | 6 |
| | ATOM | 410 | N | VAL | A | 53 | 31.712 | 7.325 | 4.777 | 1.00 | 18.75 | 7 |
| | ATOM | 411 | CA | VAL | A | 53 | 32.134 | 8.568 | 4.131 | 1.00 | 18.32 | 6 |
| | ATOM | 412 | C | VAL | A | 53 | 32.759 | 9.411 | 5.215 | 1.00 | 18.55 | 6 |
| | ATOM | 413 | O | VAL | A | 53 | 32.055 | 9.630 | 6.225 | 1.00 | 19.86 | 8 |
| 65 | ATOM | 414 | CB | VAL | A | 53 | 30.949 | 9.327 | 3.473 | 1.00 | 18.40 | 6 |
| | ATOM | 415 | CG1 | VAL | A | 53 | 31.462 | 10.680 | 2.967 | 1.00 | 20.65 | 6 |
| | ATOM | 416 | CG2 | VAL | A | 53 | 30.322 | 8.469 | 2.396 | 1.00 | 17.69 | 6 |
| | ATOM | 417 | N | SER | A | 54 | 33.913 | 9.963 | 4.996 | 1.00 | 16.45 | 7 |
| | ATOM | 418 | CA | SER | A | 54 | 34.482 | 10.911 | 5.946 | 1.00 | 20.30 | 6 |
| 70 | ATOM | 419 | C | SER | A | 54 | 34.280 | 12.349 | 5.478 | 1.00 | 21.22 | 6 |
| | ATOM | 420 | O | SER | A | 54 | 34.281 | 12.545 | 4.254 | 1.00 | 18.83 | 8 |
| | ATOM | 421 | CB | SER | A | 54 | 35.971 | 10.631 | 6.156 | 1.00 | 21.31 | 6 |
| | ATOM | 422 | OG | SER | A | 54 | 36.695 | 10.788 | 4.949 | 1.00 | 21.56 | 8 |
| | ATOM | 423 | N | ILE | A | 55 | 33.909 | 13.223 | 6.394 | 1.00 | 21.28 | 7 |
| | ATOM | 424 | CA | ILE | A | 55 | 33.699 | 14.621 | 6.108 | 1.00 | 19.86 | 6 |

-42-

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|----|
| | ATOM | 425 | C | ILE | A | 55 | 34.649 | 15.356 | 7.100 | 1.00 | 20.76 | 6 |
| | ATOM | 426 | O | ILE | A | 55 | 34.344 | 15.342 | 8.300 | 1.00 | 22.84 | 8 |
| | ATOM | 427 | CB | ILE | A | 55 | 32.273 | 15.102 | 6.291 | 1.00 | 21.61 | 6 |
| 5 | ATOM | 428 | CG1 | ILE | A | 55 | 31.333 | 14.422 | 5.255 | 1.00 | 21.20 | 6 |
| | ATOM | 429 | CG2 | ILE | A | 55 | 32.222 | 16.614 | 6.139 | 1.00 | 22.98 | 6 |
| | ATOM | 430 | CD1 | ILE | A | 55 | 29.854 | 14.691 | 5.584 | 1.00 | 24.15 | 6 |
| | ATOM | 431 | N | PHE | A | 56 | 35.723 | 15.883 | 6.577 | 1.00 | 17.70 | 7 |
| | ATOM | 432 | CA | PHE | A | 56 | 36.699 | 16.589 | 7.404 | 1.00 | 18.93 | 6 |
| 10 | ATOM | 433 | C | PHE | A | 56 | 37.459 | 17.589 | 6.579 | 1.00 | 20.83 | 6 |
| | ATOM | 434 | O | PHE | A | 56 | 38.263 | 17.314 | 5.680 | 1.00 | 21.50 | 8 |
| | ATOM | 435 | CB | PHE | A | 56 | 37.671 | 15.557 | 8.060 | 1.00 | 17.73 | 6 |
| | ATOM | 436 | CG | PHE | A | 56 | 38.721 | 16.209 | 8.950 | 1.00 | 19.66 | 6 |
| | ATOM | 437 | CD1 | PHE | A | 56 | 38.297 | 16.881 | 10.098 | 1.00 | 20.08 | 6 |
| | ATOM | 438 | CD2 | PHE | A | 56 | 40.059 | 16.144 | 8.616 | 1.00 | 20.24 | 6 |
| 15 | ATOM | 439 | CE1 | PHE | A | 56 | 39.261 | 17.479 | 10.909 | 1.00 | 19.99 | 6 |
| | ATOM | 440 | CE2 | PHE | A | 56 | 41.029 | 16.743 | 9.433 | 1.00 | 20.35 | 6 |
| | ATOM | 441 | CZ | PHE | A | 56 | 40.591 | 17.409 | 10.573 | 1.00 | 21.50 | 6 |
| | ATOM | 442 | N | VAL | A | 57 | 37.284 | 18.883 | 6.949 | 1.00 | 21.60 | 7 |
| 20 | ATOM | 443 | CA | VAL | A | 57 | 38.009 | 19.978 | 6.334 | 1.00 | 23.17 | 6 |
| | ATOM | 444 | C | VAL | A | 57 | 39.362 | 20.006 | 7.039 | 1.00 | 25.23 | 6 |
| | ATOM | 445 | O | VAL | A | 57 | 39.473 | 20.469 | 8.172 | 1.00 | 24.88 | 8 |
| | ATOM | 446 | CB | VAL | A | 57 | 37.247 | 21.325 | 6.458 | 1.00 | 23.78 | 6 |
| | ATOM | 447 | CG1 | VAL | A | 57 | 38.051 | 22.403 | 5.763 | 1.00 | 24.08 | 6 |
| 25 | ATOM | 448 | CG2 | VAL | A | 57 | 35.853 | 21.178 | 5.874 | 1.00 | 23.56 | 6 |
| | ATOM | 449 | N | ASN | A | 58 | 40.343 | 19.429 | 6.377 | 1.00 | 24.28 | 7 |
| | ATOM | 450 | CA | ASN | A | 58 | 41.667 | 19.181 | 6.907 | 1.00 | 22.31 | 6 |
| | ATOM | 451 | C | ASN | A | 58 | 42.545 | 20.385 | 6.858 | 1.00 | 23.05 | 6 |
| | ATOM | 452 | O | ASN | A | 58 | 43.072 | 20.747 | 5.806 | 1.00 | 24.44 | 8 |
| 30 | ATOM | 453 | CB | ASN | A | 58 | 42.250 | 18.045 | 6.040 | 1.00 | 21.07 | 6 |
| | ATOM | 454 | CG | ASN | A | 58 | 43.684 | 17.738 | 6.385 | 1.00 | 22.18 | 6 |
| | ATOM | 455 | OD1 | ASN | A | 58 | 44.133 | 17.942 | 7.521 | 1.00 | 23.39 | 8 |
| | ATOM | 456 | ND2 | ASN | A | 58 | 44.431 | 17.254 | 5.415 | 1.00 | 20.86 | 7 |
| | ATOM | 457 | N | PRO | A | 59 | 42.863 | 21.002 | 8.000 | 1.00 | 24.30 | 7 |
| 35 | ATOM | 458 | CA | PRO | A | 59 | 43.727 | 22.187 | 7.996 | 1.00 | 25.81 | 6 |
| | ATOM | 459 | C | PRO | A | 59 | 45.060 | 22.042 | 7.348 | 1.00 | 26.27 | 6 |
| | ATOM | 460 | O | PRO | A | 59 | 45.679 | 22.957 | 6.784 | 1.00 | 27.28 | 8 |
| | ATOM | 461 | CB | PRO | A | 59 | 43.869 | 22.509 | 9.493 | 1.00 | 24.50 | 6 |
| | ATOM | 462 | CG | PRO | A | 59 | 42.719 | 21.834 | 10.171 | 1.00 | 26.42 | 6 |
| 40 | ATOM | 463 | CD | PRO | A | 59 | 42.427 | 20.600 | 9.337 | 1.00 | 24.44 | 6 |
| | ATOM | 464 | N | MET | A | 60 | 45.602 | 20.784 | 7.391 | 1.00 | 27.24 | 7 |
| | ATOM | 465 | CA | MET | A | 60 | 46.952 | 20.529 | 6.856 | 1.00 | 28.64 | 6 |
| | ATOM | 466 | C | MET | A | 60 | 47.008 | 20.656 | 5.361 | 1.00 | 31.51 | 6 |
| | ATOM | 467 | O | MET | A | 60 | 48.101 | 20.868 | 4.822 | 1.00 | 31.68 | 8 |
| 45 | ATOM | 468 | CB | MET | A | 60 | 47.374 | 19.171 | 7.462 | 1.00 | 28.13 | 6 |
| | ATOM | 469 | CG | MET | A | 60 | 48.810 | 18.867 | 7.264 | 1.00 | 32.00 | 6 |
| | ATOM | 470 | SD | MET | A | 60 | 49.373 | 17.277 | 7.999 | 1.00 | 31.44 | 16 |
| | ATOM | 471 | CE | MET | A | 60 | 50.665 | 17.068 | 6.848 | 1.00 | 31.98 | 6 |
| | ATOM | 472 | N | GLN | A | 61 | 45.847 | 20.601 | 4.648 | 1.00 | 30.53 | 7 |
| 50 | ATOM | 473 | CA | GLN | A | 61 | 45.972 | 20.800 | 3.202 | 1.00 | 33.22 | 6 |
| | ATOM | 474 | C | GLN | A | 61 | 45.492 | 22.174 | 2.780 | 1.00 | 35.82 | 6 |
| | ATOM | 475 | O | GLN | A | 61 | 45.183 | 22.463 | 1.611 | 1.00 | 39.20 | 8 |
| | ATOM | 476 | CB | GLN | A | 61 | 45.264 | 19.567 | 2.566 | 1.00 | 31.83 | 6 |
| | ATOM | 477 | CG | GLN | A | 61 | 43.747 | 19.745 | 2.433 | 1.00 | 29.02 | 6 |
| 55 | ATOM | 478 | CD | GLN | A | 61 | 43.189 | 18.320 | 2.094 | 1.00 | 28.13 | 6 |
| | ATOM | 479 | OE1 | GLN | A | 61 | 43.302 | 17.290 | 2.731 | 1.00 | 24.18 | 8 |
| | ATOM | 480 | NE2 | GLN | A | 61 | 42.486 | 18.326 | 0.963 | 1.00 | 28.14 | 7 |
| | ATOM | 481 | N | PHE | A | 62 | 45.576 | 23.209 | 3.658 | 1.00 | 33.24 | 7 |
| | ATOM | 482 | CA | PHE | A | 62 | 45.219 | 24.574 | 3.275 | 1.00 | 33.76 | 6 |
| 60 | ATOM | 483 | C | PHE | A | 62 | 46.434 | 25.502 | 3.390 | 1.00 | 35.21 | 6 |
| | ATOM | 484 | O | PHE | A | 62 | 47.120 | 25.382 | 4.405 | 1.00 | 33.54 | 8 |
| | ATOM | 485 | CB | PHE | A | 62 | 44.138 | 25.218 | 4.136 | 1.00 | 31.27 | 6 |
| | ATOM | 486 | CG | PHE | A | 62 | 42.754 | 24.742 | 3.809 | 1.00 | 30.27 | 6 |
| | ATOM | 487 | CD1 | PHE | A | 62 | 42.301 | 23.528 | 4.291 | 1.00 | 29.03 | 6 |
| 65 | ATOM | 488 | CD2 | PHE | A | 62 | 41.930 | 25.486 | 2.975 | 1.00 | 29.79 | 6 |
| | ATOM | 489 | CE1 | PHE | A | 62 | 41.037 | 23.065 | 3.956 | 1.00 | 28.62 | 6 |
| | ATOM | 490 | CE2 | PHE | A | 62 | 40.682 | 25.043 | 2.637 | 1.00 | 28.83 | 6 |
| | ATOM | 491 | CZ | PHE | A | 62 | 40.223 | 23.823 | 3.112 | 1.00 | 28.44 | 6 |
| | ATOM | 492 | N | ASP | A | 63 | 46.598 | 26.394 | 2.439 | 1.00 | 40.06 | 7 |
| 70 | ATOM | 493 | CA | ASP | A | 63 | 47.689 | 27.339 | 2.350 | 1.00 | 42.93 | 6 |
| | ATOM | 494 | C | ASP | A | 63 | 47.787 | 28.342 | 3.485 | 1.00 | 44.06 | 6 |
| | ATOM | 495 | O | ASP | A | 63 | 48.906 | 28.726 | 3.827 | 1.00 | 43.96 | 8 |
| | ATOM | 496 | CB | ASP | A | 63 | 47.575 | 28.206 | 1.085 | 1.00 | 47.09 | 6 |
| | ATOM | 497 | CG | ASP | A | 63 | 47.423 | 27.434 | -0.198 | 1.00 | 51.39 | 6 |
| | ATOM | 498 | OD1 | ASP | A | 63 | 47.397 | 26.169 | -0.162 | 1.00 | 54.46 | 8 |

-43-

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 499 | OD2 | ASP | A | 63 | 47.317 | 28.098 | -1.257 | 1.00 | 52.58 | 8 |
| | ATOM | 500 | N | ARG | A | 64 | 46.669 | 28.845 | 3.990 | 1.00 | 43.31 | 7 |
| | ATOM | 501 | CA | ARG | A | 64 | 46.717 | 29.795 | 5.095 | 1.00 | 44.44 | 6 |
| 5 | ATOM | 502 | C | ARG | A | 64 | 45.451 | 29.635 | 5.923 | 1.00 | 41.86 | 6 |
| | ATOM | 503 | O | ARG | A | 64 | 44.424 | 29.201 | 5.428 | 1.00 | 38.21 | 8 |
| | ATOM | 504 | CB | ARG | A | 64 | 46.808 | 31.240 | 4.660 | 1.00 | 47.55 | 6 |
| | ATOM | 505 | CG | ARG | A | 64 | 48.161 | 31.803 | 4.295 | 1.00 | 52.46 | 6 |
| | ATOM | 506 | CD | ARG | A | 64 | 47.938 | 33.125 | 3.520 | 1.00 | 55.58 | 6 |
| 10 | ATOM | 507 | NE | ARG | A | 64 | 47.067 | 32.875 | 2.441 | 1.00 | 58.62 | 7 |
| | ATOM | 508 | CZ | ARG | A | 64 | 46.215 | 32.846 | 1.486 | 1.00 | 60.36 | 6 |
| | ATOM | 509 | NH1 | ARG | A | 64 | 45.436 | 33.900 | 1.230 | 1.00 | 62.10 | 7 |
| | ATOM | 510 | NH2 | ARG | A | 64 | 46.118 | 31.748 | 0.742 | 1.00 | 60.56 | 7 |
| | ATOM | 511 | N | PRO | A | 65 | 45.506 | 30.080 | 7.169 | 1.00 | 41.07 | 7 |
| 15 | ATOM | 512 | CA | PRO | A | 65 | 44.375 | 30.002 | 8.068 | 1.00 | 41.23 | 6 |
| | ATOM | 513 | C | PRO | A | 65 | 43.127 | 30.709 | 7.584 | 1.00 | 41.03 | 6 |
| | ATOM | 514 | O | PRO | A | 65 | 42.000 | 30.258 | 7.847 | 1.00 | 39.31 | 8 |
| | ATOM | 515 | CB | PRO | A | 65 | 44.911 | 30.622 | 9.356 | 1.00 | 42.70 | 6 |
| | ATOM | 516 | CG | PRO | A | 65 | 46.398 | 30.368 | 9.281 | 1.00 | 43.00 | 6 |
| 20 | ATOM | 517 | CD | PRO | A | 65 | 46.709 | 30.642 | 7.823 | 1.00 | 42.34 | 6 |
| | ATOM | 518 | N | GLU | A | 66 | 43.274 | 31.789 | 6.810 | 1.00 | 41.59 | 7 |
| | ATOM | 519 | CA | GLU | A | 66 | 42.070 | 32.514 | 6.362 | 1.00 | 42.96 | 6 |
| | ATOM | 520 | C | GLU | A | 66 | 41.347 | 31.757 | 5.259 | 1.00 | 40.61 | 6 |
| | ATOM | 521 | O | GLU | A | 66 | 40.120 | 31.853 | 5.153 | 1.00 | 38.18 | 8 |
| 25 | ATOM | 522 | CB | GLU | A | 66 | 42.463 | 33.934 | 5.932 | 1.00 | 48.02 | 6 |
| | ATOM | 523 | CG | GLU | A | 66 | 43.670 | 33.931 | 5.016 | 1.00 | 54.67 | 6 |
| | ATOM | 524 | CD | GLU | A | 66 | 44.083 | 35.290 | 4.503 | 1.00 | 59.02 | 6 |
| | ATOM | 525 | OE1 | GLU | A | 66 | 44.156 | 36.244 | 5.323 | 1.00 | 62.04 | 8 |
| | ATOM | 526 | OE2 | GLU | A | 66 | 44.334 | 35.389 | 3.276 | 1.00 | 60.81 | 8 |
| 30 | ATOM | 527 | N | ASP | A | 67 | 42.108 | 30.969 | 4.481 | 1.00 | 38.50 | 7 |
| | ATOM | 528 | CA | ASP | A | 67 | 41.447 | 30.178 | 3.439 | 1.00 | 37.14 | 6 |
| | ATOM | 529 | C | ASP | A | 67 | 40.655 | 29.082 | 4.122 | 1.00 | 34.07 | 6 |
| | ATOM | 530 | O | ASP | A | 67 | 39.529 | 28.761 | 3.792 | 1.00 | 30.58 | 8 |
| | ATOM | 531 | CB | ASP | A | 67 | 42.413 | 29.550 | 2.449 | 1.00 | 41.16 | 6 |
| 35 | ATOM | 532 | CG | ASP | A | 67 | 43.388 | 30.540 | 1.846 | 1.00 | 44.61 | 6 |
| | ATOM | 533 | OD1 | ASP | A | 67 | 43.068 | 31.742 | 1.741 | 1.00 | 46.57 | 8 |
| | ATOM | 534 | OD2 | ASP | A | 67 | 44.487 | 30.073 | 1.482 | 1.00 | 47.46 | 8 |
| | ATOM | 535 | N | LEU | A | 68 | 41.286 | 28.452 | 5.142 | 1.00 | 31.94 | 7 |
| | ATOM | 536 | CA | LEU | A | 68 | 40.581 | 27.433 | 5.887 | 1.00 | 30.62 | 6 |
| 40 | ATOM | 537 | C | LEU | A | 68 | 39.303 | 27.981 | 6.477 | 1.00 | 30.54 | 6 |
| | ATOM | 538 | O | LEU | A | 68 | 38.243 | 27.345 | 6.533 | 1.00 | 30.35 | 8 |
| | ATOM | 539 | CB | LEU | A | 68 | 41.523 | 26.893 | 7.001 | 1.00 | 29.74 | 6 |
| | ATOM | 540 | CG | LEU | A | 68 | 40.908 | 25.958 | 8.016 | 1.00 | 30.11 | 6 |
| | ATOM | 541 | CD1 | LEU | A | 68 | 40.510 | 24.577 | 7.474 | 1.00 | 30.95 | 6 |
| 45 | ATOM | 542 | CD2 | LEU | A | 68 | 41.899 | 25.712 | 9.149 | 1.00 | 31.60 | 6 |
| | ATOM | 543 | N | ALA | A | 69 | 39.345 | 29.225 | 7.012 | 1.00 | 29.90 | 7 |
| | ATOM | 544 | CA | ALA | A | 69 | 38.146 | 29.740 | 7.662 | 1.00 | 32.87 | 6 |
| | ATOM | 545 | C | ALA | A | 69 | 37.021 | 29.993 | 6.663 | 1.00 | 34.82 | 6 |
| | ATOM | 546 | O | ALA | A | 69 | 35.855 | 29.854 | 7.018 | 1.00 | 35.59 | 8 |
| 50 | ATOM | 547 | CB | ALA | A | 69 | 38.487 | 31.030 | 8.425 | 1.00 | 32.66 | 6 |
| | ATOM | 548 | N | ARG | A | 70 | 37.345 | 30.321 | 5.431 | 1.00 | 34.63 | 7 |
| | ATOM | 549 | CA | ARG | A | 70 | 36.337 | 30.625 | 4.423 | 1.00 | 37.34 | 6 |
| | ATOM | 550 | C | ARG | A | 70 | 35.777 | 29.350 | 3.803 | 1.00 | 36.74 | 6 |
| | ATOM | 551 | O | ARG | A | 70 | 34.726 | 29.502 | 3.165 | 1.00 | 35.73 | 8 |
| 55 | ATOM | 552 | CB | ARG | A | 70 | 36.923 | 31.526 | 3.334 | 1.00 | 38.93 | 6 |
| | ATOM | 553 | CG | ARG | A | 70 | 37.284 | 32.923 | 3.813 | 1.00 | 41.54 | 6 |
| | ATOM | 554 | CD | ARG | A | 70 | 37.555 | 33.855 | 2.643 | 1.00 | 43.19 | 6 |
| | ATOM | 555 | NE | ARG | A | 70 | 38.731 | 33.447 | 1.880 | 1.00 | 47.13 | 7 |
| | ATOM | 556 | CZ | ARG | A | 70 | 39.977 | 33.789 | 2.190 | 1.00 | 47.82 | 6 |
| 60 | ATOM | 557 | NH1 | ARG | A | 70 | 40.213 | 34.544 | 3.252 | 1.00 | 51.37 | 7 |
| | ATOM | 558 | NH2 | ARG | A | 70 | 40.984 | 33.371 | 1.435 | 1.00 | 48.98 | 7 |
| | ATOM | 559 | N | TYR | A | 71 | 36.419 | 28.197 | 3.875 | 1.00 | 32.87 | 7 |
| | ATOM | 560 | CA | TYR | A | 71 | 35.941 | 26.999 | 3.187 | 1.00 | 31.99 | 6 |
| | ATOM | 561 | C | TYR | A | 71 | 34.522 | 26.700 | 3.578 | 1.00 | 30.54 | 6 |
| 65 | ATOM | 562 | O | TYR | A | 71 | 34.125 | 26.714 | 4.739 | 1.00 | 30.28 | 8 |
| | ATOM | 563 | CB | TYR | A | 71 | 36.927 | 25.840 | 3.502 | 1.00 | 29.15 | 6 |
| | ATOM | 564 | CG | TYR | A | 71 | 36.753 | 24.730 | 2.482 | 1.00 | 29.96 | 6 |
| | ATOM | 565 | CD1 | TYR | A | 71 | 37.363 | 24.753 | 1.233 | 1.00 | 30.99 | 6 |
| | ATOM | 566 | CD2 | TYR | A | 71 | 35.931 | 23.658 | 2.815 | 1.00 | 29.82 | 6 |
| 70 | ATOM | 567 | CE1 | TYR | A | 71 | 37.166 | 23.667 | 0.356 | 1.00 | 33.09 | 6 |
| | ATOM | 568 | CE2 | TYR | A | 71 | 35.713 | 22.625 | 1.927 | 1.00 | 31.04 | 6 |
| | ATOM | 569 | CZ | TYR | A | 71 | 36.332 | 22.650 | 0.702 | 1.00 | 31.47 | 6 |
| | ATOM | 570 | OH | TYR | A | 71 | 36.163 | 21.647 | -0.214 | 1.00 | 34.74 | 8 |
| | ATOM | 571 | N | PRO | A | 72 | 33.687 | 26.356 | 2.591 | 1.00 | 33.76 | 7 |
| | ATOM | 572 | CA | PRO | A | 72 | 32.271 | 26.095 | 2.809 | 1.00 | 35.62 | 6 |

-44-

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|----|
| | ATOM | 573 | C | PRO | A | 72 | 31.987 | 24.932 | 3.712 | 1.00 | 36.23 | 6 |
| | ATOM | 574 | O | PRO | A | 72 | 32.552 | 23.855 | 3.521 | 1.00 | 37.45 | 8 |
| | ATOM | 575 | CB | PRO | A | 72 | 31.695 | 25.904 | 1.408 | 1.00 | 36.05 | 6 |
| 5 | ATOM | 576 | CG | PRO | A | 72 | 32.853 | 25.628 | 0.524 | 1.00 | 36.68 | 6 |
| | ATOM | 577 | CD | PRO | A | 72 | 34.044 | 26.284 | 1.155 | 1.00 | 35.26 | 6 |
| | ATOM | 578 | N | ARG | A | 73 | 31.114 | 25.089 | 4.705 | 1.00 | 35.24 | 7 |
| | ATOM | 579 | CA | ARG | A | 73 | 30.752 | 23.978 | 5.580 | 1.00 | 35.44 | 6 |
| | ATOM | 580 | C | ARG | A | 73 | 29.254 | 23.808 | 5.446 | 1.00 | 36.32 | 6 |
| 10 | ATOM | 581 | O | ARG | A | 73 | 28.544 | 24.827 | 5.569 | 1.00 | 36.64 | 8 |
| | ATOM | 582 | CB | ARG | A | 73 | 31.232 | 24.214 | 7.012 | 1.00 | 37.96 | 6 |
| | ATOM | 583 | CG | ARG | A | 73 | 32.778 | 24.055 | 6.985 | 1.00 | 38.27 | 6 |
| | ATOM | 584 | CD | ARG | A | 73 | 33.433 | 24.599 | 8.180 | 1.00 | 39.86 | 6 |
| | ATOM | 585 | NE | ARG | A | 73 | 34.854 | 24.417 | 8.347 | 1.00 | 37.69 | 7 |
| 15 | ATOM | 586 | CZ | ARG | A | 73 | 35.799 | 25.216 | 7.876 | 1.00 | 38.63 | 6 |
| | ATOM | 587 | NH1 | ARG | A | 73 | 37.047 | 24.918 | 8.212 | 1.00 | 36.16 | 7 |
| | ATOM | 588 | NH2 | ARG | A | 73 | 35.534 | 26.279 | 7.132 | 1.00 | 38.20 | 7 |
| | ATOM | 589 | N | THR | A | 74 | 28.763 | 22.645 | 5.057 | 1.00 | 34.43 | 7 |
| | ATOM | 590 | CA | THR | A | 74 | 27.358 | 22.363 | 4.859 | 1.00 | 34.04 | 6 |
| 20 | ATOM | 591 | C | THR | A | 74 | 27.033 | 20.953 | 5.354 | 1.00 | 32.80 | 6 |
| | ATOM | 592 | O | THR | A | 74 | 26.421 | 20.107 | 4.689 | 1.00 | 31.08 | 8 |
| | ATOM | 593 | CB | THR | A | 74 | 26.856 | 22.409 | 3.403 | 1.00 | 36.39 | 6 |
| | ATOM | 594 | OG1 | THR | A | 74 | 27.567 | 21.394 | 2.652 | 1.00 | 38.24 | 8 |
| | ATOM | 595 | CG2 | THR | A | 74 | 27.020 | 23.800 | 2.776 | 1.00 | 37.30 | 6 |
| 25 | ATOM | 596 | N | LEU | A | 75 | 27.405 | 20.714 | 6.616 | 1.00 | 31.90 | 7 |
| | ATOM | 597 | CA | LEU | A | 75 | 27.234 | 19.377 | 7.168 | 1.00 | 30.80 | 6 |
| | ATOM | 598 | C | LEU | A | 75 | 25.818 | 18.900 | 7.129 | 1.00 | 30.32 | 6 |
| | ATOM | 599 | O | LEU | A | 75 | 25.595 | 17.716 | 6.815 | 1.00 | 29.31 | 8 |
| | ATOM | 600 | CB | LEU | A | 75 | 27.865 | 19.401 | 8.605 | 1.00 | 32.17 | 6 |
| 30 | ATOM | 601 | CG | LEU | A | 75 | 27.986 | 18.001 | 9.219 | 1.00 | 33.15 | 6 |
| | ATOM | 602 | CD1 | LEU | A | 75 | 28.985 | 17.154 | 8.420 | 1.00 | 33.59 | 6 |
| | ATOM | 603 | CD2 | LEU | A | 75 | 28.401 | 18.093 | 10.663 | 1.00 | 32.87 | 6 |
| | ATOM | 604 | N | GLN | A | 76 | 24.793 | 19.692 | 7.502 | 1.00 | 29.90 | 7 |
| | ATOM | 605 | CA | GLN | A | 76 | 23.429 | 19.175 | 7.436 | 1.00 | 31.72 | 6 |
| 35 | ATOM | 606 | C | GLN | A | 76 | 23.040 | 18.695 | 6.054 | 1.00 | 28.82 | 6 |
| | ATOM | 607 | O | GLN | A | 76 | 22.449 | 17.626 | 5.924 | 1.00 | 30.69 | 8 |
| | ATOM | 608 | CB | GLN | A | 76 | 22.423 | 20.270 | 7.881 | 1.00 | 34.78 | 6 |
| | ATOM | 609 | CG | GLN | A | 76 | 21.016 | 19.720 | 8.042 | 1.00 | 40.38 | 6 |
| | ATOM | 610 | CD | GLN | A | 76 | 20.095 | 20.836 | 8.524 | 1.00 | 45.28 | 6 |
| 40 | ATOM | 611 | OE1 | GLN | A | 76 | 19.111 | 21.196 | 7.859 | 1.00 | 48.24 | 8 |
| | ATOM | 612 | NE2 | GLN | A | 76 | 20.453 | 21.402 | 9.677 | 1.00 | 47.35 | 7 |
| | ATOM | 613 | N | GLU | A | 77 | 23.274 | 19.493 | 5.023 | 1.00 | 26.49 | 7 |
| | ATOM | 614 | CA | GLU | A | 77 | 22.946 | 19.111 | 3.656 | 1.00 | 27.35 | 6 |
| | ATOM | 615 | C | GLU | A | 77 | 23.777 | 17.906 | 3.193 | 1.00 | 27.59 | 6 |
| 45 | ATOM | 616 | O | GLU | A | 77 | 23.263 | 17.064 | 2.463 | 1.00 | 27.03 | 8 |
| | ATOM | 617 | CB | GLU | A | 77 | 23.227 | 20.280 | 2.718 | 1.00 | 28.83 | 6 |
| | ATOM | 618 | CG | GLU | A | 77 | 22.722 | 19.997 | 1.302 | 1.00 | 32.09 | 6 |
| | ATOM | 619 | N | ASP | A | 78 | 25.048 | 17.886 | 3.617 | 1.00 | 26.66 | 7 |
| | ATOM | 620 | CA | ASP | A | 78 | 25.875 | 16.706 | 3.239 | 1.00 | 26.91 | 6 |
| 50 | ATOM | 621 | C | ASP | A | 78 | 25.226 | 15.431 | 3.735 | 1.00 | 26.68 | 6 |
| | ATOM | 622 | O | ASP | A | 78 | 25.042 | 14.448 | 3.018 | 1.00 | 24.38 | 8 |
| | ATOM | 623 | CB | ASP | A | 78 | 27.275 | 16.820 | 3.796 | 1.00 | 25.18 | 6 |
| | ATOM | 624 | CG | ASP | A | 78 | 28.116 | 17.931 | 3.332 | 1.00 | 28.50 | 6 |
| | ATOM | 625 | OD1 | ASP | A | 78 | 27.681 | 18.573 | 2.312 | 1.00 | 28.92 | 8 |
| 55 | ATOM | 626 | OD2 | ASP | A | 78 | 29.179 | 18.397 | 3.774 | 1.00 | 29.90 | 8 |
| | ATOM | 627 | N | CYS | A | 79 | 24.883 | 15.488 | 5.051 | 1.00 | 27.85 | 7 |
| | ATOM | 628 | CA | CYS | A | 79 | 24.304 | 14.292 | 5.666 | 1.00 | 30.04 | 6 |
| | ATOM | 629 | C | CYS | A | 79 | 22.949 | 13.894 | 5.111 | 1.00 | 29.71 | 6 |
| | ATOM | 630 | O | CYS | A | 79 | 22.684 | 12.715 | 4.944 | 1.00 | 29.58 | 8 |
| 60 | ATOM | 631 | CB | CYS | A | 79 | 24.188 | 14.507 | 7.183 | 1.00 | 31.67 | 6 |
| | ATOM | 632 | SG | CYS | A | 79 | 25.844 | 14.386 | 7.916 | 1.00 | 33.92 | 16 |
| | ATOM | 633 | N | GLU | A | 80 | 22.134 | 14.874 | 4.734 | 1.00 | 30.93 | 7 |
| | ATOM | 634 | CA | GLU | A | 80 | 20.899 | 14.555 | 4.007 | 1.00 | 32.01 | 6 |
| | ATOM | 635 | C | GLU | A | 80 | 21.197 | 13.812 | 2.705 | 1.00 | 29.17 | 6 |
| 65 | ATOM | 636 | O | GLU | A | 80 | 20.524 | 12.822 | 2.413 | 1.00 | 29.08 | 8 |
| | ATOM | 637 | CB | GLU | A | 80 | 20.135 | 15.852 | 3.756 | 1.00 | 36.34 | 6 |
| | ATOM | 638 | CG | GLU | A | 80 | 19.379 | 16.349 | 4.985 | 1.00 | 43.73 | 6 |
| | ATOM | 639 | CD | GLU | A | 80 | 18.700 | 17.700 | 4.818 | 1.00 | 48.86 | 6 |
| | ATOM | 640 | OE1 | GLU | A | 80 | 18.432 | 18.156 | 3.670 | 1.00 | 51.62 | 8 |
| 70 | ATOM | 641 | OE2 | GLU | A | 80 | 18.442 | 18.338 | 5.884 | 1.00 | 51.33 | 8 |
| | ATOM | 642 | N | LYS | A | 81 | 22.175 | 14.264 | 1.921 | 1.00 | 26.79 | 7 |
| | ATOM | 643 | CA | LYS | A | 81 | 22.522 | 13.581 | 0.676 | 1.00 | 27.73 | 6 |
| | ATOM | 644 | C | LYS | A | 81 | 23.067 | 12.161 | 0.921 | 1.00 | 27.62 | 6 |
| | ATOM | 645 | O | LYS | A | 81 | 22.686 | 11.291 | 0.147 | 1.00 | 25.90 | 8 |
| | ATOM | 646 | CB | LYS | A | 81 | 23.541 | 14.390 | -0.112 | 1.00 | 27.61 | 6 |

-45-

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 647 | CG | LYS | A | 81 | 23.036 | 15.708 | -0.702 | 1.00 | 27.05 | 6 |
| | ATOM | 648 | CD | LYS | A | 81 | 24.149 | 16.381 | -1.485 | 1.00 | 29.23 | 6 |
| | ATOM | 649 | CE | LYS | A | 81 | 23.586 | 17.726 | -1.958 | 1.00 | 31.40 | 6 |
| 5 | ATOM | 650 | NZ | LYS | A | 81 | 24.290 | 18.189 | -3.180 | 1.00 | 33.21 | 7 |
| | ATOM | 651 | N | LEU | A | 82 | 23.941 | 12.067 | 1.932 | 1.00 | 25.01 | 7 |
| | ATOM | 652 | CA | LEU | A | 82 | 24.428 | 10.653 | 2.208 | 1.00 | 25.50 | 6 |
| | ATOM | 653 | C | LEU | A | 82 | 23.359 | 9.729 | 2.719 | 1.00 | 24.46 | 6 |
| | ATOM | 654 | O | LEU | A | 82 | 23.296 | 8.571 | 2.335 | 1.00 | 25.35 | 8 |
| 10 | ATOM | 655 | CB | LEU | A | 82 | 25.616 | 10.767 | 3.179 | 1.00 | 24.87 | 6 |
| | ATOM | 656 | CG | LEU | A | 82 | 26.765 | 11.600 | 2.627 | 1.00 | 25.74 | 6 |
| | ATOM | 657 | CD1 | LEU | A | 82 | 27.854 | 11.923 | 3.663 | 1.00 | 24.08 | 6 |
| | ATOM | 658 | CD2 | LEU | A | 82 | 27.412 | 10.853 | 1.463 | 1.00 | 24.64 | 6 |
| | ATOM | 659 | N | ASN | A | 83 | 22.437 | 10.262 | 3.549 | 1.00 | 27.59 | 7 |
| 15 | ATOM | 660 | CA | ASN | A | 83 | 21.352 | 9.467 | 4.081 | 1.00 | 29.62 | 6 |
| | ATOM | 661 | C | ASN | A | 83 | 20.400 | 9.086 | 2.941 | 1.00 | 31.66 | 6 |
| | ATOM | 662 | O | ASN | A | 83 | 20.066 | 7.899 | 2.966 | 1.00 | 31.60 | 8 |
| | ATOM | 663 | CB | ASN | A | 83 | 20.649 | 10.212 | 5.205 | 1.00 | 32.77 | 6 |
| | ATOM | 664 | CG | ASN | A | 83 | 19.718 | 9.324 | 6.010 | 1.00 | 37.49 | 6 |
| 20 | ATOM | 665 | OD1 | ASN | A | 83 | 18.788 | 9.898 | 6.588 | 1.00 | 42.54 | 8 |
| | ATOM | 666 | ND2 | ASN | A | 83 | 19.899 | 8.019 | 6.093 | 1.00 | 37.69 | 7 |
| | ATOM | 667 | N | LYS | A | 84 | 20.176 | 9.954 | 1.933 | 1.00 | 31.56 | 7 |
| | ATOM | 668 | CA | LYS | A | 84 | 19.397 | 9.440 | 0.781 | 1.00 | 33.04 | 6 |
| | ATOM | 669 | C | LYS | A | 84 | 20.155 | 8.440 | -0.069 | 1.00 | 34.14 | 6 |
| 25 | ATOM | 670 | O | LYS | A | 84 | 19.531 | 7.661 | -0.824 | 1.00 | 34.69 | 8 |
| | ATOM | 671 | CB | LYS | A | 84 | 18.915 | 10.637 | -0.071 | 1.00 | 36.71 | 6 |
| | ATOM | 672 | CG | LYS | A | 84 | 17.639 | 11.350 | 0.339 | 1.00 | 42.14 | 6 |
| | ATOM | 673 | CD | LYS | A | 84 | 17.457 | 12.707 | -0.355 | 1.00 | 45.16 | 6 |
| | ATOM | 674 | CE | LYS | A | 84 | 16.334 | 13.494 | 0.303 | 1.00 | 48.19 | 6 |
| 30 | ATOM | 675 | NZ | LYS | A | 84 | 16.337 | 14.928 | -0.105 | 1.00 | 50.51 | 7 |
| | ATOM | 676 | N | ARG | A | 85 | 21.483 | 8.305 | 0.021 | 1.00 | 34.32 | 7 |
| | ATOM | 677 | CA | ARG | A | 85 | 22.276 | 7.344 | -0.773 | 1.00 | 33.70 | 6 |
| | ATOM | 678 | C | ARG | A | 85 | 22.620 | 6.057 | -0.050 | 1.00 | 34.60 | 6 |
| | ATOM | 679 | O | ARG | A | 85 | 23.358 | 5.112 | -0.377 | 1.00 | 36.33 | 8 |
| 35 | ATOM | 680 | CB | ARG | A | 85 | 23.529 | 8.099 | -1.166 | 1.00 | 34.84 | 6 |
| | ATOM | 681 | CG | ARG | A | 85 | 24.040 | 7.946 | -2.583 | 1.00 | 36.24 | 6 |
| | ATOM | 682 | CD | ARG | A | 85 | 23.177 | 8.780 | -3.502 | 1.00 | 37.79 | 6 |
| | ATOM | 683 | NE | ARG | A | 85 | 23.549 | 8.555 | -4.891 | 1.00 | 36.63 | 7 |
| | ATOM | 684 | CZ | ARG | A | 85 | 23.122 | 9.364 | -5.853 | 1.00 | 37.76 | 6 |
| 40 | ATOM | 685 | NH1 | ARG | A | 85 | 22.368 | 10.397 | -5.507 | 1.00 | 38.88 | 7 |
| | ATOM | 686 | NH2 | ARG | A | 85 | 23.473 | 9.117 | -7.100 | 1.00 | 37.39 | 7 |
| | ATOM | 687 | N | LYS | A | 86 | 21.948 | 5.940 | 1.093 | 1.00 | 33.51 | 7 |
| | ATOM | 688 | CA | LYS | A | 86 | 21.983 | 4.881 | 2.059 | 1.00 | 34.48 | 6 |
| | ATOM | 689 | C | LYS | A | 86 | 23.404 | 4.563 | 2.503 | 1.00 | 32.25 | 6 |
| 45 | ATOM | 690 | O | LYS | A | 86 | 23.823 | 3.405 | 2.516 | 1.00 | 34.37 | 8 |
| | ATOM | 691 | CB | LYS | A | 86 | 21.290 | 3.624 | 1.477 | 1.00 | 37.47 | 6 |
| | ATOM | 692 | CG | LYS | A | 86 | 19.862 | 3.957 | 1.034 | 1.00 | 42.40 | 6 |
| | ATOM | 693 | CD | LYS | A | 86 | 18.990 | 4.373 | 2.205 | 1.00 | 46.88 | 6 |
| | ATOM | 694 | CE | LYS | A | 86 | 18.857 | 3.256 | 3.233 | 1.00 | 50.03 | 6 |
| 50 | ATOM | 695 | NZ | LYS | A | 86 | 18.397 | 3.827 | 4.543 | 1.00 | 52.47 | 7 |
| | ATOM | 696 | N | VAL | A | 87 | 24.138 | 5.595 | 2.885 | 1.00 | 29.97 | 7 |
| | ATOM | 697 | CA | VAL | A | 87 | 25.490 | 5.405 | 3.428 | 1.00 | 26.05 | 6 |
| | ATOM | 698 | C | VAL | A | 87 | 25.390 | 4.849 | 4.829 | 1.00 | 28.43 | 6 |
| | ATOM | 699 | O | VAL | A | 87 | 24.498 | 5.233 | 5.587 | 1.00 | 26.14 | 8 |
| 55 | ATOM | 700 | CB | VAL | A | 87 | 26.199 | 6.749 | 3.397 | 1.00 | 26.58 | 6 |
| | ATOM | 701 | CG1 | VAL | A | 87 | 27.425 | 6.848 | 4.304 | 1.00 | 23.69 | 6 |
| | ATOM | 702 | CG2 | VAL | A | 87 | 26.640 | 7.063 | 1.961 | 1.00 | 25.53 | 6 |
| | ATOM | 703 | N | ASP | A | 88 | 26.274 | 3.947 | 5.231 | 1.00 | 25.06 | 7 |
| | ATOM | 704 | CA | ASP | A | 88 | 26.163 | 3.320 | 6.552 | 1.00 | 27.11 | 6 |
| 60 | ATOM | 705 | C | ASP | A | 88 | 26.718 | 4.129 | 7.696 | 1.00 | 26.68 | 6 |
| | ATOM | 706 | O | ASP | A | 88 | 26.108 | 4.221 | 8.763 | 1.00 | 27.00 | 8 |
| | ATOM | 707 | CB | ASP | A | 88 | 26.899 | 1.986 | 6.461 | 1.00 | 29.00 | 6 |
| | ATOM | 708 | CG | ASP | A | 88 | 26.332 | 1.114 | 5.377 | 1.00 | 31.90 | 6 |
| | ATOM | 709 | OD1 | ASP | A | 88 | 25.301 | 0.444 | 5.714 | 1.00 | 34.25 | 8 |
| 65 | ATOM | 710 | OD2 | ASP | A | 88 | 26.819 | 1.060 | 4.237 | 1.00 | 30.16 | 8 |
| | ATOM | 711 | N | LEU | A | 89 | 27.798 | 4.864 | 7.483 | 1.00 | 21.05 | 7 |
| | ATOM | 712 | CA | LEU | A | 89 | 28.448 | 5.620 | 8.532 | 1.00 | 22.89 | 6 |
| | ATOM | 713 | C | LEU | A | 89 | 29.085 | 6.879 | 7.997 | 1.00 | 25.24 | 6 |
| | ATOM | 714 | O | LEU | A | 89 | 29.775 | 6.771 | 6.967 | 1.00 | 24.36 | 8 |
| 70 | ATOM | 715 | CB | LEU | A | 89 | 29.561 | 4.723 | 9.069 | 1.00 | 27.61 | 6 |
| | ATOM | 716 | CG | LEU | A | 89 | 30.275 | 5.099 | 10.342 | 1.00 | 31.35 | 6 |
| | ATOM | 717 | CD1 | LEU | A | 89 | 30.916 | 3.857 | 10.963 | 1.00 | 34.98 | 6 |
| | ATOM | 718 | CD2 | LEU | A | 89 | 31.363 | 6.137 | 10.099 | 1.00 | 33.01 | 6 |
| | ATOM | 719 | N | VAL | A | 90 | 28.910 | 7.987 | 8.677 | 1.00 | 22.49 | 7 |
| | ATOM | 720 | CA | VAL | A | 90 | 29.577 | 9.200 | 8.296 | 1.00 | 23.34 | 6 |

-46-

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|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| | ATOM | 721 | C | VAL | A | 90 | 30.551 | 9.518 | 9.431 | 1.00 | 24.94 | 6 |
| | ATOM | 722 | O | VAL | A | 90 | 30.041 | 9.581 | 10.575 | 1.00 | 25.44 | 8 |
| | ATOM | 723 | CB | VAL | A | 90 | 28.602 | 10.366 | 8.153 | 1.00 | 21.61 | 6 |
| 5 | ATOM | 724 | CG1 | VAL | A | 90 | 29.294 | 11.692 | 7.966 | 1.00 | 23.24 | 6 |
| | ATOM | 725 | CG2 | VAL | A | 90 | 27.695 | 10.065 | 6.945 | 1.00 | 24.01 | 6 |
| | ATOM | 726 | N | PHE | A | 91 | 31.819 | 9.736 | 9.120 | 1.00 | 20.62 | 7 |
| | ATOM | 727 | CA | PHE | A | 91 | 32.779 | 10.106 | 10.131 | 1.00 | 21.25 | 6 |
| | ATOM | 728 | C | PHE | A | 91 | 33.008 | 11.589 | 9.966 | 1.00 | 22.65 | 6 |
| 10 | ATOM | 729 | O | PHE | A | 91 | 33.612 | 12.028 | 8.957 | 1.00 | 20.89 | 8 |
| | ATOM | 730 | CB | PHE | A | 91 | 34.059 | 9.254 | 9.968 | 1.00 | 20.01 | 6 |
| | ATOM | 731 | CG | PHE | A | 91 | 35.181 | 9.639 | 10.897 | 1.00 | 20.02 | 6 |
| | ATOM | 732 | CD1 | PHE | A | 91 | 34.954 | 9.716 | 12.277 | 1.00 | 20.82 | 6 |
| | ATOM | 733 | CD2 | PHE | A | 91 | 36.465 | 9.830 | 10.421 | 1.00 | 21.38 | 6 |
| 15 | ATOM | 734 | CE1 | PHE | A | 91 | 36.004 | 10.045 | 13.150 | 1.00 | 21.05 | 6 |
| | ATOM | 735 | CE2 | PHE | A | 91 | 37.503 | 10.196 | 11.281 | 1.00 | 23.76 | 6 |
| | ATOM | 736 | CZ | PHE | A | 91 | 37.261 | 10.233 | 12.631 | 1.00 | 21.99 | 6 |
| | ATOM | 737 | N | ALA | A | 92 | 32.580 | 12.382 | 10.985 | 1.00 | 23.09 | 7 |
| | ATOM | 738 | CA | ALA | A | 92 | 32.750 | 13.824 | 10.898 | 1.00 | 23.04 | 6 |
| 20 | ATOM | 739 | C | ALA | A | 92 | 33.406 | 14.387 | 12.142 | 1.00 | 24.15 | 6 |
| | ATOM | 740 | O | ALA | A | 92 | 32.699 | 14.986 | 12.979 | 1.00 | 24.45 | 8 |
| | ATOM | 741 | CB | ALA | A | 92 | 31.368 | 14.496 | 10.717 | 1.00 | 23.41 | 6 |
| | ATOM | 742 | N | PRO | A | 93 | 34.701 | 14.252 | 12.284 | 1.00 | 23.10 | 7 |
| | ATOM | 743 | CA | PRO | A | 93 | 35.387 | 14.638 | 13.507 | 1.00 | 21.87 | 6 |
| 25 | ATOM | 744 | C | PRO | A | 93 | 35.695 | 16.093 | 13.560 | 1.00 | 23.67 | 6 |
| | ATOM | 745 | O | PRO | A | 93 | 35.740 | 16.790 | 12.510 | 1.00 | 24.71 | 8 |
| | ATOM | 746 | CB | PRO | A | 93 | 36.687 | 13.798 | 13.426 | 1.00 | 21.94 | 6 |
| | ATOM | 747 | CG | PRO | A | 93 | 37.002 | 13.904 | 11.930 | 1.00 | 23.58 | 6 |
| | ATOM | 748 | CD | PRO | A | 93 | 35.643 | 13.553 | 11.336 | 1.00 | 21.29 | 6 |
| 30 | ATOM | 749 | N | SER | A | 94 | 35.940 | 16.664 | 14.752 | 1.00 | 23.63 | 7 |
| | ATOM | 750 | CA | SER | A | 94 | 36.447 | 18.022 | 14.812 | 1.00 | 26.17 | 6 |
| | ATOM | 751 | C | SER | A | 94 | 37.939 | 18.117 | 14.561 | 1.00 | 26.12 | 6 |
| | ATOM | 752 | O | SER | A | 94 | 38.700 | 17.126 | 14.588 | 1.00 | 25.24 | 8 |
| | ATOM | 753 | CB | SER | A | 94 | 36.151 | 18.617 | 16.207 | 1.00 | 26.90 | 6 |
| 35 | ATOM | 754 | OG | SER | A | 94 | 36.930 | 17.871 | 17.168 | 1.00 | 27.23 | 8 |
| | ATOM | 755 | N | VAL | A | 95 | 38.487 | 19.308 | 14.308 | 1.00 | 25.69 | 7 |
| | ATOM | 756 | CA | VAL | A | 95 | 39.900 | 19.519 | 14.115 | 1.00 | 25.50 | 6 |
| | ATOM | 757 | C | VAL | A | 95 | 40.639 | 19.107 | 15.409 | 1.00 | 28.17 | 6 |
| | ATOM | 758 | O | VAL | A | 95 | 41.692 | 18.475 | 15.307 | 1.00 | 27.54 | 8 |
| 40 | ATOM | 759 | CB | VAL | A | 95 | 40.319 | 20.963 | 13.788 | 1.00 | 27.40 | 6 |
| | ATOM | 760 | CG1 | VAL | A | 95 | 41.808 | 21.236 | 13.929 | 1.00 | 27.91 | 6 |
| | ATOM | 761 | CG2 | VAL | A | 95 | 39.873 | 21.263 | 12.346 | 1.00 | 26.36 | 6 |
| | ATOM | 762 | N | LYS | A | 96 | 40.047 | 19.405 | 16.570 | 1.00 | 26.82 | 7 |
| | ATOM | 763 | CA | LYS | A | 96 | 40.718 | 18.994 | 17.823 | 1.00 | 28.89 | 6 |
| 45 | ATOM | 764 | C | LYS | A | 96 | 40.773 | 17.474 | 17.962 | 1.00 | 28.61 | 6 |
| | ATOM | 765 | O | LYS | A | 96 | 41.723 | 16.951 | 18.539 | 1.00 | 27.95 | 8 |
| | ATOM | 766 | CB | LYS | A | 96 | 40.013 | 19.550 | 19.066 | 1.00 | 29.19 | 6 |
| | ATOM | 767 | N | GLU | A | 97 | 39.756 | 16.765 | 17.486 | 1.00 | 28.36 | 7 |
| | ATOM | 768 | CA | GLU | A | 97 | 39.748 | 15.295 | 17.583 | 1.00 | 29.80 | 6 |
| 50 | ATOM | 769 | C | GLU | A | 97 | 40.830 | 14.674 | 16.708 | 1.00 | 29.13 | 6 |
| | ATOM | 770 | O | GLU | A | 97 | 41.565 | 13.752 | 17.126 | 1.00 | 29.24 | 8 |
| | ATOM | 771 | CB | GLU | A | 97 | 38.365 | 14.782 | 17.214 | 1.00 | 29.05 | 6 |
| | ATOM | 772 | CG | GLU | A | 97 | 38.194 | 13.265 | 17.303 | 1.00 | 28.83 | 6 |
| | ATOM | 773 | CD | GLU | A | 97 | 38.133 | 12.796 | 18.762 | 1.00 | 30.81 | 6 |
| 55 | ATOM | 774 | OE1 | GLU | A | 97 | 38.046 | 13.687 | 19.649 | 1.00 | 32.00 | 8 |
| | ATOM | 775 | OE2 | GLU | A | 97 | 38.132 | 11.592 | 19.080 | 1.00 | 28.32 | 8 |
| | ATOM | 776 | N | ILE | A | 98 | 41.066 | 15.194 | 15.516 | 1.00 | 26.74 | 7 |
| | ATOM | 777 | CA | ILE | A | 98 | 42.110 | 14.673 | 14.641 | 1.00 | 24.88 | 6 |
| | ATOM | 778 | C | ILE | A | 98 | 43.483 | 15.219 | 14.955 | 1.00 | 26.67 | 6 |
| 60 | ATOM | 779 | O | ILE | A | 98 | 44.485 | 14.459 | 14.852 | 1.00 | 24.09 | 8 |
| | ATOM | 780 | CB | ILE | A | 98 | 41.817 | 14.972 | 13.147 | 1.00 | 23.79 | 6 |
| | ATOM | 781 | CG1 | ILE | A | 98 | 40.483 | 14.337 | 12.789 | 1.00 | 22.35 | 6 |
| | ATOM | 782 | CG2 | ILE | A | 98 | 42.971 | 14.486 | 12.252 | 1.00 | 22.39 | 6 |
| | ATOM | 783 | CD1 | ILE | A | 98 | 40.431 | 12.804 | 12.865 | 1.00 | 24.57 | 6 |
| 65 | ATOM | 784 | N | TYR | A | 99 | 43.603 | 16.493 | 15.375 | 1.00 | 24.39 | 7 |
| | ATOM | 785 | CA | TYR | A | 99 | 44.886 | 17.127 | 15.585 | 1.00 | 26.57 | 6 |
| | ATOM | 786 | C | TYR | A | 99 | 44.917 | 17.788 | 16.978 | 1.00 | 26.98 | 6 |
| | ATOM | 787 | O | TYR | A | 99 | 44.959 | 18.984 | 17.080 | 1.00 | 29.92 | 8 |
| | ATOM | 788 | CB | TYR | A | 99 | 45.244 | 18.185 | 14.514 | 1.00 | 24.58 | 6 |
| 70 | ATOM | 789 | CG | TYR | A | 99 | 45.318 | 17.673 | 13.080 | 1.00 | 24.59 | 6 |
| | ATOM | 790 | CD1 | TYR | A | 99 | 44.461 | 18.086 | 12.085 | 1.00 | 23.63 | 6 |
| | ATOM | 791 | CD2 | TYR | A | 99 | 46.371 | 16.838 | 12.709 | 1.00 | 23.01 | 6 |
| | ATOM | 792 | CE1 | TYR | A | 99 | 44.573 | 17.677 | 10.760 | 1.00 | 23.55 | 6 |
| | ATOM | 793 | CE2 | TYR | A | 99 | 46.491 | 16.358 | 11.405 | 1.00 | 25.75 | 6 |
| | ATOM | 794 | CZ | TYR | A | 99 | 45.593 | 16.773 | 10.447 | 1.00 | 24.33 | 6 |

-47-

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|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 795 | OH | TYR | A | 99 | 45.814 | 16.340 | 9.160 | 1.00 | 22.62 | 8 |
| | ATOM | 796 | N | PRO | A | 100 | 44.891 | 17.004 | 18.020 | 1.00 | 29.54 | 7 |
| | ATOM | 797 | CA | PRO | A | 100 | 44.819 | 17.563 | 19.401 | 1.00 | 30.81 | 6 |
| | ATOM | 798 | C | PRO | A | 100 | 46.024 | 18.411 | 19.723 | 1.00 | 33.04 | 6 |
| 5 | ATOM | 799 | O | PRO | A | 100 | 45.855 | 19.351 | 20.545 | 1.00 | 34.95 | 8 |
| | ATOM | 800 | CB | PRO | A | 100 | 44.652 | 16.358 | 20.291 | 1.00 | 32.03 | 6 |
| | ATOM | 801 | CG | PRO | A | 100 | 45.376 | 15.277 | 19.517 | 1.00 | 31.65 | 6 |
| | ATOM | 802 | CD | PRO | A | 100 | 44.894 | 15.532 | 18.081 | 1.00 | 29.86 | 6 |
| 10 | ATOM | 803 | N | ASN | A | 101 | 47.177 | 18.234 | 19.116 | 1.00 | 30.09 | 7 |
| | ATOM | 804 | CA | ASN | A | 101 | 48.364 | 19.030 | 19.406 | 1.00 | 29.38 | 6 |
| | ATOM | 805 | C | ASN | A | 101 | 48.732 | 19.925 | 18.258 | 1.00 | 28.34 | 6 |
| | ATOM | 806 | O | ASN | A | 101 | 49.831 | 20.474 | 18.133 | 1.00 | 29.73 | 8 |
| | ATOM | 807 | CB | ASN | A | 101 | 49.573 | 18.111 | 19.726 | 1.00 | 32.63 | 6 |
| | ATOM | 808 | CG | ASN | A | 101 | 49.136 | 17.044 | 20.693 | 1.00 | 32.29 | 6 |
| 15 | ATOM | 809 | OD1 | ASN | A | 101 | 49.095 | 15.839 | 20.358 | 1.00 | 35.88 | 8 |
| | ATOM | 810 | ND2 | ASN | A | 101 | 48.725 | 17.480 | 21.868 | 1.00 | 33.54 | 7 |
| | ATOM | 811 | N | GLY | A | 102 | 47.764 | 20.158 | 17.344 | 1.00 | 28.24 | 7 |
| | ATOM | 812 | CA | GLY | A | 102 | 48.018 | 20.969 | 16.192 | 1.00 | 28.54 | 6 |
| | ATOM | 813 | C | GLY | A | 102 | 48.572 | 20.122 | 15.054 | 1.00 | 28.73 | 6 |
| 20 | ATOM | 814 | O | GLY | A | 102 | 48.848 | 18.918 | 15.212 | 1.00 | 28.80 | 8 |
| | ATOM | 815 | N | THR | A | 103 | 48.797 | 20.786 | 13.929 | 1.00 | 28.45 | 7 |
| | ATOM | 816 | CA | THR | A | 103 | 49.271 | 20.035 | 12.755 | 1.00 | 27.44 | 6 |
| | ATOM | 817 | C | THR | A | 103 | 50.751 | 20.121 | 12.584 | 1.00 | 27.75 | 6 |
| | ATOM | 818 | O | THR | A | 103 | 51.419 | 19.270 | 11.979 | 1.00 | 28.24 | 8 |
| 25 | ATOM | 819 | CB | THR | A | 103 | 48.585 | 20.545 | 11.461 | 1.00 | 28.39 | 6 |
| | ATOM | 820 | OG1 | THR | A | 103 | 49.011 | 21.911 | 11.287 | 1.00 | 29.31 | 8 |
| | ATOM | 821 | CG2 | THR | A | 103 | 47.081 | 20.410 | 11.575 | 1.00 | 25.68 | 6 |
| | ATOM | 822 | N | GLU | A | 104 | 51.410 | 21.114 | 13.189 | 1.00 | 26.94 | 7 |
| 30 | ATOM | 823 | CA | GLU | A | 104 | 52.843 | 21.274 | 12.953 | 1.00 | 30.65 | 6 |
| | ATOM | 824 | C | GLU | A | 104 | 53.682 | 20.149 | 13.572 | 1.00 | 27.87 | 6 |
| | ATOM | 825 | O | GLU | A | 104 | 54.755 | 19.902 | 13.010 | 1.00 | 30.98 | 8 |
| | ATOM | 826 | CB | GLU | A | 104 | 53.353 | 22.617 | 13.515 | 1.00 | 34.13 | 6 |
| | ATOM | 827 | CG | GLU | A | 104 | 52.613 | 23.746 | 12.784 | 1.00 | 40.22 | 6 |
| | ATOM | 828 | CD | GLU | A | 104 | 51.319 | 24.211 | 13.411 | 1.00 | 44.21 | 6 |
| 35 | ATOM | 829 | OE1 | GLU | A | 104 | 50.583 | 23.551 | 14.187 | 1.00 | 42.68 | 8 |
| | ATOM | 830 | OE2 | GLU | A | 104 | 50.972 | 25.409 | 13.090 | 1.00 | 48.99 | 8 |
| | ATOM | 831 | N | THR | A | 105 | 53.210 | 19.618 | 14.686 | 1.00 | 24.87 | 7 |
| | ATOM | 832 | CA | THR | A | 105 | 54.112 | 18.554 | 15.230 | 1.00 | 25.37 | 6 |
| | ATOM | 833 | C | THR | A | 105 | 53.586 | 17.170 | 14.962 | 1.00 | 24.14 | 6 |
| 40 | ATOM | 834 | O | THR | A | 105 | 54.100 | 16.162 | 15.504 | 1.00 | 23.64 | 8 |
| | ATOM | 835 | CB | THR | A | 105 | 54.301 | 18.763 | 16.735 | 1.00 | 24.29 | 6 |
| | ATOM | 836 | OG1 | THR | A | 105 | 53.037 | 18.773 | 17.363 | 1.00 | 27.37 | 8 |
| | ATOM | 837 | CG2 | THR | A | 105 | 55.020 | 20.098 | 16.999 | 1.00 | 27.01 | 6 |
| 45 | ATOM | 838 | N | HIS | A | 106 | 52.456 | 17.094 | 14.251 | 1.00 | 22.37 | 7 |
| | ATOM | 839 | CA | HIS | A | 106 | 51.897 | 15.760 | 13.955 | 1.00 | 22.53 | 6 |
| | ATOM | 840 | C | HIS | A | 106 | 52.748 | 15.031 | 12.927 | 1.00 | 20.08 | 6 |
| | ATOM | 841 | O | HIS | A | 106 | 53.289 | 15.552 | 11.960 | 1.00 | 22.95 | 8 |
| | ATOM | 842 | CB | HIS | A | 106 | 50.457 | 15.962 | 13.432 | 1.00 | 20.21 | 6 |
| 50 | ATOM | 843 | CG | HIS | A | 106 | 49.534 | 14.791 | 13.386 | 1.00 | 19.83 | 6 |
| | ATOM | 844 | ND1 | HIS | A | 106 | 49.650 | 13.883 | 12.350 | 1.00 | 19.73 | 7 |
| | ATOM | 845 | CD2 | HIS | A | 106 | 48.484 | 14.387 | 14.112 | 1.00 | 18.64 | 6 |
| | ATOM | 846 | CE1 | HIS | A | 106 | 48.695 | 13.003 | 12.509 | 1.00 | 17.48 | 6 |
| | ATOM | 847 | NE2 | HIS | A | 106 | 47.914 | 13.255 | 13.533 | 1.00 | 19.68 | 7 |
| | ATOM | 848 | N | THR | A | 107 | 52.772 | 13.689 | 13.062 | 1.00 | 21.05 | 7 |
| 55 | ATOM | 849 | CA | THR | A | 107 | 53.466 | 12.840 | 12.117 | 1.00 | 20.53 | 6 |
| | ATOM | 850 | C | THR | A | 107 | 52.946 | 13.066 | 10.697 | 1.00 | 20.02 | 6 |
| | ATOM | 851 | O | THR | A | 107 | 51.730 | 13.301 | 10.684 | 1.00 | 20.34 | 8 |
| | ATOM | 852 | CB | THR | A | 107 | 53.232 | 11.366 | 12.525 | 1.00 | 21.22 | 6 |
| 60 | ATOM | 853 | OG1 | THR | A | 107 | 53.808 | 11.185 | 13.848 | 1.00 | 22.21 | 8 |
| | ATOM | 854 | CG2 | THR | A | 107 | 53.856 | 10.364 | 11.540 | 1.00 | 21.83 | 6 |
| | ATOM | 855 | N | TYR | A | 108 | 53.769 | 13.113 | 9.699 | 1.00 | 20.01 | 7 |
| | ATOM | 856 | CA | TYR | A | 108 | 53.224 | 13.286 | 8.347 | 1.00 | 22.77 | 6 |
| | ATOM | 857 | C | TYR | A | 108 | 53.796 | 12.231 | 7.405 | 1.00 | 21.91 | 6 |
| 65 | ATOM | 858 | O | TYR | A | 108 | 54.794 | 11.532 | 7.605 | 1.00 | 19.88 | 8 |
| | ATOM | 859 | CB | TYR | A | 108 | 53.505 | 14.695 | 7.860 | 1.00 | 23.51 | 6 |
| | ATOM | 860 | CG | TYR | A | 108 | 54.978 | 15.076 | 7.762 | 1.00 | 24.54 | 6 |
| | ATOM | 861 | CD1 | TYR | A | 108 | 55.707 | 14.832 | 6.624 | 1.00 | 25.82 | 6 |
| | ATOM | 862 | CD2 | TYR | A | 108 | 55.623 | 15.677 | 8.857 | 1.00 | 26.49 | 6 |
| 70 | ATOM | 863 | CE1 | TYR | A | 108 | 57.051 | 15.146 | 6.526 | 1.00 | 29.12 | 6 |
| | ATOM | 864 | CE2 | TYR | A | 108 | 56.970 | 16.024 | 8.781 | 1.00 | 29.06 | 6 |
| | ATOM | 865 | CZ | TYR | A | 108 | 57.664 | 15.733 | 7.631 | 1.00 | 29.44 | 6 |
| | ATOM | 866 | OH | TYR | A | 108 | 58.995 | 16.072 | 7.478 | 1.00 | 32.47 | 8 |
| | ATOM | 867 | N | VAL | A | 109 | 53.052 | 12.125 | 6.280 | 1.00 | 19.53 | 7 |
| | ATOM | 868 | CA | VAL | A | 109 | 53.431 | 11.213 | 5.194 | 1.00 | 20.38 | 6 |

-48-

| | | | | | | | | | | | | |
|----|------|-----|-----|-----|---|-----|--------|--------|---------|------|-------|----|
| | ATOM | 869 | C | VAL | A | 109 | 53.653 | 12.022 | 3.954 | 1.00 | 24.73 | 6 |
| | ATOM | 870 | O | VAL | A | 109 | 52.756 | 12.811 | 3.553 | 1.00 | 23.81 | 8 |
| | ATOM | 871 | CB | VAL | A | 109 | 52.263 | 10.230 | 4.964 | 1.00 | 20.04 | 6 |
| 5 | ATOM | 872 | CG1 | VAL | A | 109 | 52.619 | 9.362 | 3.731 | 1.00 | 23.57 | 6 |
| | ATOM | 873 | CG2 | VAL | A | 109 | 51.946 | 9.420 | 6.209 | 1.00 | 17.72 | 6 |
| | ATOM | 874 | N | ASP | A | 110 | 54.753 | 11.885 | 3.237 | 1.00 | 25.18 | 7 |
| | ATOM | 875 | CA | ASP | A | 110 | 55.054 | 12.663 | 2.047 | 1.00 | 28.26 | 6 |
| | ATOM | 876 | C | ASP | A | 110 | 55.453 | 11.784 | 0.881 | 1.00 | 25.00 | 6 |
| 10 | ATOM | 877 | O | ASP | A | 110 | 56.220 | 10.815 | 1.006 | 1.00 | 23.50 | 8 |
| | ATOM | 878 | CB | ASP | A | 110 | 56.199 | 13.596 | 2.383 | 1.00 | 34.46 | 6 |
| | ATOM | 879 | CG | ASP | A | 110 | 56.031 | 15.027 | 1.970 | 1.00 | 42.11 | 6 |
| | ATOM | 880 | OD1 | ASP | A | 110 | 56.945 | 15.774 | 2.403 | 1.00 | 48.30 | 8 |
| | ATOM | 881 | OD2 | ASP | A | 110 | 55.098 | 15.496 | 1.290 | 1.00 | 46.79 | 8 |
| 15 | ATOM | 882 | N | VAL | A | 111 | 54.851 | 11.964 | -0.272 | 1.00 | 24.14 | 7 |
| | ATOM | 883 | CA | VAL | A | 111 | 55.111 | 11.236 | -1.493 | 1.00 | 23.80 | 6 |
| | ATOM | 884 | C | VAL | A | 111 | 56.023 | 12.085 | -2.363 | 1.00 | 24.56 | 6 |
| | ATOM | 885 | O | VAL | A | 111 | 55.572 | 13.037 | -3.027 | 1.00 | 25.12 | 8 |
| | ATOM | 886 | CB | VAL | A | 111 | 53.771 | 10.929 | -2.218 | 1.00 | 23.25 | 6 |
| 20 | ATOM | 887 | CG1 | VAL | A | 111 | 54.020 | 10.068 | -3.456 | 1.00 | 22.00 | 6 |
| | ATOM | 888 | CG2 | VAL | A | 111 | 52.810 | 10.285 | -1.246 | 1.00 | 22.35 | 6 |
| | ATOM | 889 | N | PRO | A | 112 | 57.278 | 11.687 | -2.453 | 1.00 | 26.28 | 7 |
| | ATOM | 890 | CA | PRO | A | 112 | 58.274 | 12.438 | -3.222 | 1.00 | 27.97 | 6 |
| | ATOM | 891 | C | PRO | A | 112 | 57.906 | 12.619 | -4.650 | 1.00 | 30.72 | 6 |
| 25 | ATOM | 892 | O | PRO | A | 112 | 57.272 | 11.711 | -5.253 | 1.00 | 30.37 | 8 |
| | ATOM | 893 | CB | PRO | A | 112 | 59.532 | 11.573 | -3.106 | 1.00 | 27.29 | 6 |
| | ATOM | 894 | CG | PRO | A | 112 | 59.413 | 10.926 | -1.769 | 1.00 | 27.60 | 6 |
| | ATOM | 895 | CD | PRO | A | 112 | 57.905 | 10.536 | -1.762 | 1.00 | 24.64 | 6 |
| | ATOM | 896 | N | GLY | A | 113 | 58.211 | 13.800 | -5.209 | 1.00 | 30.66 | 7 |
| 30 | ATOM | 897 | CA | GLY | A | 113 | 57.940 | 14.000 | -6.614 | 1.00 | 32.72 | 6 |
| | ATOM | 898 | C | GLY | A | 113 | 56.543 | 14.464 | -6.926 | 1.00 | 31.39 | 6 |
| | ATOM | 899 | O | GLY | A | 113 | 56.346 | 15.614 | -7.280 | 1.00 | 30.61 | 8 |
| | ATOM | 900 | N | LEU | A | 114 | 55.558 | 13.575 | -6.772 | 1.00 | 27.67 | 7 |
| | ATOM | 901 | CA | LEU | A | 114 | 54.192 | 13.922 | -7.023 | 1.00 | 28.50 | 6 |
| 35 | ATOM | 902 | C | LEU | A | 114 | 53.677 | 15.086 | -6.186 | 1.00 | 29.37 | 6 |
| | ATOM | 903 | O | LEU | A | 114 | 52.810 | 15.829 | -6.657 | 1.00 | 33.05 | 8 |
| | ATOM | 904 | CB | LEU | A | 114 | 53.283 | 12.710 | -6.702 | 1.00 | 29.66 | 6 |
| | ATOM | 905 | CG | LEU | A | 114 | 53.515 | 11.551 | -7.669 | 1.00 | 31.75 | 6 |
| | ATOM | 906 | CD1 | LEU | A | 114 | 52.703 | 10.351 | -7.233 | 1.00 | 31.73 | 6 |
| 40 | ATOM | 907 | CD2 | LEU | A | 114 | 53.134 | 11.977 | -9.059 | 1.00 | 35.50 | 6 |
| | ATOM | 908 | N | SER | A | 115 | 54.161 | 15.180 | -4.965 | 1.00 | 26.50 | 7 |
| | ATOM | 909 | CA | SER | A | 115 | 53.664 | 16.206 | -4.063 | 1.00 | 27.52 | 6 |
| | ATOM | 910 | C | SER | A | 115 | 54.245 | 17.582 | -4.400 | 1.00 | 30.00 | 6 |
| | ATOM | 911 | O | SER | A | 115 | 53.590 | 18.536 | -3.932 | 1.00 | 28.18 | 8 |
| 45 | ATOM | 912 | CB | SER | A | 115 | 53.978 | 15.885 | -2.599 | 1.00 | 25.46 | 6 |
| | ATOM | 913 | OG | SER | A | 115 | 55.407 | 15.846 | -2.464 | 1.00 | 30.73 | 8 |
| | ATOM | 914 | N | THR | A | 116 | 55.312 | 17.617 | -5.177 | 1.00 | 30.25 | 7 |
| | ATOM | 915 | CA | THR | A | 116 | 55.884 | 18.969 | -5.426 | 1.00 | 32.64 | 6 |
| | ATOM | 916 | C | THR | A | 116 | 55.854 | 19.345 | -6.870 | 1.00 | 33.28 | 6 |
| 50 | ATOM | 917 | O | THR | A | 116 | 56.516 | 20.337 | -7.260 | 1.00 | 37.48 | 8 |
| | ATOM | 918 | CB | THR | A | 116 | 57.318 | 19.018 | -4.839 | 1.00 | 31.68 | 6 |
| | ATOM | 919 | OG1 | THR | A | 116 | 58.066 | 17.923 | -5.419 | 1.00 | 33.81 | 8 |
| | ATOM | 920 | CG2 | THR | A | 116 | 57.348 | 18.863 | -3.344 | 1.00 | 30.91 | 6 |
| | ATOM | 921 | N | MET | A | 117 | 55.075 | 18.691 | -7.725 | 1.00 | 34.70 | 7 |
| 55 | ATOM | 922 | CA | MET | A | 117 | 54.978 | 19.104 | -9.116 | 1.00 | 36.76 | 6 |
| | ATOM | 923 | C | MET | A | 117 | 53.599 | 19.679 | -9.408 | 1.00 | 35.12 | 6 |
| | ATOM | 924 | O | MET | A | 117 | 52.722 | 19.561 | -8.569 | 1.00 | 34.04 | 8 |
| | ATOM | 925 | CB | MET | A | 117 | 55.258 | 17.952 | -10.067 | 1.00 | 38.70 | 6 |
| | ATOM | 926 | CG | MET | A | 117 | 54.494 | 16.690 | -9.707 | 1.00 | 41.51 | 6 |
| 60 | ATOM | 927 | SD | MET | A | 117 | 55.327 | 15.244 | -10.403 | 1.00 | 45.13 | 16 |
| | ATOM | 928 | CE | MET | A | 117 | 55.643 | 15.848 | -12.065 | 1.00 | 43.90 | 6 |
| | ATOM | 929 | N | LEU | A | 118 | 53.449 | 20.272 | -10.578 | 1.00 | 35.18 | 7 |
| | ATOM | 930 | CA | LEU | A | 118 | 52.173 | 20.846 | -10.995 | 1.00 | 36.73 | 6 |
| | ATOM | 931 | C | LEU | A | 118 | 51.570 | 21.660 | -9.877 | 1.00 | 36.48 | 6 |
| 65 | ATOM | 932 | O | LEU | A | 118 | 52.236 | 22.552 | -9.330 | 1.00 | 36.60 | 8 |
| | ATOM | 933 | CB | LEU | A | 118 | 51.252 | 19.706 | -11.478 | 1.00 | 38.22 | 6 |
| | ATOM | 934 | CG | LEU | A | 118 | 51.872 | 18.829 | -12.571 | 1.00 | 39.36 | 6 |
| | ATOM | 935 | CD1 | LEU | A | 118 | 51.001 | 17.679 | -13.051 | 1.00 | 41.36 | 6 |
| | ATOM | 936 | CD2 | LEU | A | 118 | 52.194 | 19.710 | -13.783 | 1.00 | 41.80 | 6 |
| 70 | ATOM | 937 | N | GLU | A | 119 | 50.329 | 21.339 | -9.481 | 1.00 | 38.80 | 7 |
| | ATOM | 938 | CA | GLU | A | 119 | 49.645 | 22.049 | -8.411 | 1.00 | 37.83 | 6 |
| | ATOM | 939 | C | GLU | A | 119 | 50.401 | 22.088 | -7.102 | 1.00 | 38.27 | 6 |
| | ATOM | 940 | O | GLU | A | 119 | 50.416 | 23.101 | -6.393 | 1.00 | 38.36 | 8 |
| | ATOM | 941 | CB | GLU | A | 119 | 48.255 | 21.394 | -8.141 | 1.00 | 41.10 | 6 |
| | ATOM | 942 | CG | GLU | A | 119 | 47.470 | 22.109 | -7.049 | 1.00 | 41.69 | 6 |

-49-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 943 | CD | GLU | A | 119 | 46.082 | 21.559 | -6.784 | 1.00 | 44.93 | 6 |
| | ATOM | 944 | OE1 | GLU | A | 119 | 45.654 | 20.593 | -7.453 | 1.00 | 40.85 | 8 |
| | ATOM | 945 | OE2 | GLU | A | 119 | 45.379 | 22.098 | -5.892 | 1.00 | 45.21 | 8 |
| 5 | ATOM | 946 | N | GLY | A | 120 | 51.165 | 21.031 | -6.805 | 1.00 | 35.61 | 7 |
| | ATOM | 947 | CA | GLY | A | 120 | 51.945 | 20.951 | -5.595 | 1.00 | 33.60 | 6 |
| | ATOM | 948 | C | GLY | A | 120 | 53.033 | 22.013 | -5.540 | 1.00 | 34.42 | 6 |
| | ATOM | 949 | O | GLY | A | 120 | 53.390 | 22.405 | -4.437 | 1.00 | 36.33 | 8 |
| | ATOM | 950 | N | ALA | A | 121 | 53.588 | 22.394 | -6.677 | 1.00 | 35.01 | 7 |
| 10 | ATOM | 951 | CA | ALA | A | 121 | 54.622 | 23.437 | -6.741 | 1.00 | 35.93 | 6 |
| | ATOM | 952 | C | ALA | A | 121 | 54.069 | 24.789 | -6.295 | 1.00 | 39.30 | 6 |
| | ATOM | 953 | O | ALA | A | 121 | 54.752 | 25.536 | -5.588 | 1.00 | 40.98 | 8 |
| | ATOM | 954 | CB | ALA | A | 121 | 55.189 | 23.547 | -8.150 | 1.00 | 32.29 | 6 |
| | ATOM | 955 | N | SER | A | 122 | 52.818 | 25.124 | -6.644 | 1.00 | 41.40 | 7 |
| 15 | ATOM | 956 | CA | SER | A | 122 | 52.261 | 26.415 | -6.226 | 1.00 | 44.40 | 6 |
| | ATOM | 957 | C | SER | A | 122 | 51.626 | 26.354 | -4.849 | 1.00 | 45.24 | 6 |
| | ATOM | 958 | O | SER | A | 122 | 51.056 | 27.328 | -4.339 | 1.00 | 44.99 | 8 |
| | ATOM | 959 | CB | SER | A | 122 | 51.226 | 26.909 | -7.241 | 1.00 | 45.02 | 6 |
| | ATOM | 960 | OG | SER | A | 122 | 50.178 | 25.972 | -7.432 | 1.00 | 46.98 | 8 |
| 20 | ATOM | 961 | N | ARG | A | 123 | 51.634 | 25.169 | -4.197 | 1.00 | 45.65 | 7 |
| | ATOM | 962 | CA | ARG | A | 123 | 51.045 | 24.991 | -2.876 | 1.00 | 44.81 | 6 |
| | ATOM | 963 | C | ARG | A | 123 | 51.908 | 24.083 | -2.006 | 1.00 | 44.93 | 6 |
| | ATOM | 964 | O | ARG | A | 123 | 51.557 | 22.916 | -1.788 | 1.00 | 44.88 | 8 |
| | ATOM | 965 | CB | ARG | A | 123 | 49.631 | 24.419 | -2.992 | 1.00 | 45.81 | 6 |
| 25 | ATOM | 966 | CG | ARG | A | 123 | 48.629 | 25.367 | -3.630 | 1.00 | 46.85 | 6 |
| | ATOM | 967 | CD | ARG | A | 123 | 47.248 | 24.736 | -3.714 | 1.00 | 50.24 | 6 |
| | ATOM | 968 | NE | ARG | A | 123 | 46.466 | 24.971 | -2.504 | 1.00 | 52.21 | 7 |
| | ATOM | 969 | CZ | ARG | A | 123 | 45.271 | 24.437 | -2.271 | 1.00 | 52.64 | 6 |
| | ATOM | 970 | NH1 | ARG | A | 123 | 44.718 | 23.633 | -3.169 | 1.00 | 52.96 | 7 |
| 30 | ATOM | 971 | NH2 | ARG | A | 123 | 44.633 | 24.708 | -1.141 | 1.00 | 53.34 | 7 |
| | ATOM | 972 | N | PRO | A | 124 | 52.717 | 24.827 | -1.604 | 1.00 | 44.27 | 7 |
| | ATOM | 973 | CA | PRO | A | 124 | 53.669 | 24.219 | -0.725 | 1.00 | 43.54 | 6 |
| | ATOM | 974 | C | PRO | A | 124 | 53.075 | 23.501 | 0.473 | 1.00 | 43.43 | 6 |
| | ATOM | 975 | O | PRO | A | 124 | 52.427 | 24.264 | 1.223 | 1.00 | 44.21 | 8 |
| 35 | ATOM | 976 | CB | PRO | A | 124 | 54.534 | 25.391 | -0.224 | 1.00 | 43.61 | 6 |
| | ATOM | 977 | CG | PRO | A | 124 | 54.396 | 26.439 | -1.257 | 1.00 | 44.17 | 6 |
| | ATOM | 978 | CD | PRO | A | 124 | 52.971 | 26.302 | -1.746 | 1.00 | 44.92 | 6 |
| | ATOM | 979 | N | GLY | A | 125 | 53.248 | 21.897 | 0.840 | 1.00 | 39.19 | 7 |
| | ATOM | 980 | CA | GLY | A | 125 | 52.585 | 21.453 | 2.061 | 1.00 | 34.50 | 6 |
| 40 | ATOM | 981 | C | GLY | A | 125 | 51.230 | 20.789 | 1.809 | 1.00 | 32.64 | 6 |
| | ATOM | 982 | O | GLY | A | 125 | 50.689 | 20.112 | 2.669 | 1.00 | 32.97 | 8 |
| | ATOM | 983 | N | HIS | A | 126 | 50.594 | 21.246 | 0.725 | 1.00 | 29.92 | 7 |
| | ATOM | 984 | CA | HIS | A | 126 | 49.259 | 20.776 | 0.381 | 1.00 | 29.41 | 6 |
| | ATOM | 985 | C | HIS | A | 126 | 49.186 | 19.276 | 0.256 | 1.00 | 29.27 | 6 |
| 45 | ATOM | 986 | O | HIS | A | 126 | 48.500 | 18.637 | 1.071 | 1.00 | 29.29 | 8 |
| | ATOM | 987 | CB | HIS | A | 126 | 48.782 | 21.451 | -0.934 | 1.00 | 29.82 | 6 |
| | ATOM | 988 | CG | HIS | A | 126 | 47.453 | 20.951 | -1.417 | 1.00 | 30.87 | 6 |
| | ATOM | 989 | ND1 | HIS | A | 126 | 46.254 | 21.263 | -0.790 | 1.00 | 32.42 | 7 |
| | ATOM | 990 | CD2 | HIS | A | 126 | 47.135 | 20.149 | -2.435 | 1.00 | 30.12 | 6 |
| 50 | ATOM | 991 | CE1 | HIS | A | 126 | 45.274 | 20.643 | -1.373 | 1.00 | 30.81 | 6 |
| | ATOM | 992 | NE2 | HIS | A | 126 | 45.765 | 19.970 | -2.384 | 1.00 | 33.87 | 7 |
| | ATOM | 993 | N | PHE | A | 127 | 49.882 | 18.662 | -0.698 | 1.00 | 25.60 | 7 |
| | ATOM | 994 | CA | PHE | A | 127 | 49.770 | 17.232 | -0.922 | 1.00 | 25.14 | 6 |
| | ATOM | 995 | C | PHE | A | 127 | 50.320 | 16.367 | 0.221 | 1.00 | 24.25 | 6 |
| 55 | ATOM | 996 | O | PHE | A | 127 | 49.733 | 15.332 | 0.490 | 1.00 | 23.64 | 8 |
| | ATOM | 997 | CB | PHE | A | 127 | 50.454 | 16.851 | -2.264 | 1.00 | 25.66 | 6 |
| | ATOM | 998 | CG | PHE | A | 127 | 49.518 | 17.250 | -3.398 | 1.00 | 24.51 | 6 |
| | ATOM | 999 | CD1 | PHE | A | 127 | 49.899 | 18.239 | -4.302 | 1.00 | 25.76 | 6 |
| | ATOM | 1000 | CD2 | PHE | A | 127 | 48.239 | 16.734 | -3.509 | 1.00 | 26.77 | 6 |
| 60 | ATOM | 1001 | CE1 | PHE | A | 127 | 49.026 | 18.618 | -5.301 | 1.00 | 27.57 | 6 |
| | ATOM | 1002 | CE2 | PHE | A | 127 | 47.381 | 17.086 | -4.518 | 1.00 | 27.77 | 6 |
| | ATOM | 1003 | CZ | PHE | A | 127 | 47.749 | 18.072 | -5.444 | 1.00 | 28.09 | 6 |
| | ATOM | 1004 | N | ARG | A | 128 | 51.218 | 16.966 | 1.006 | 1.00 | 24.68 | 7 |
| | ATOM | 1005 | CA | ARG | A | 128 | 51.645 | 16.377 | 2.261 | 1.00 | 23.44 | 6 |
| 65 | ATOM | 1006 | C | ARG | A | 128 | 50.408 | 16.283 | 3.155 | 1.00 | 21.06 | 6 |
| | ATOM | 1007 | O | ARG | A | 128 | 50.190 | 15.299 | 3.852 | 1.00 | 22.12 | 8 |
| | ATOM | 1008 | CB | ARG | A | 128 | 52.743 | 17.172 | 2.975 | 1.00 | 26.43 | 6 |
| | ATOM | 1009 | CG | ARG | A | 128 | 53.051 | 16.644 | 4.371 | 1.00 | 28.47 | 6 |
| | ATOM | 1010 | CD | ARG | A | 128 | 54.116 | 17.508 | 5.117 | 1.00 | 27.86 | 6 |
| 70 | ATOM | 1011 | NE | ARG | A | 128 | 55.345 | 17.336 | 4.336 | 1.00 | 31.98 | 7 |
| | ATOM | 1012 | CZ | ARG | A | 128 | 56.526 | 17.872 | 4.699 | 1.00 | 36.93 | 6 |
| | ATOM | 1013 | NH1 | ARG | A | 128 | 56.631 | 18.561 | 5.825 | 1.00 | 34.28 | 7 |
| | ATOM | 1014 | NH2 | ARG | A | 128 | 57.586 | 17.630 | 3.912 | 1.00 | 38.42 | 7 |
| | ATOM | 1015 | N | GLY | A | 129 | 49.588 | 17.337 | 3.161 | 1.00 | 21.21 | 7 |
| | ATOM | 1016 | CA | GLY | A | 129 | 48.391 | 17.274 | 4.018 | 1.00 | 21.01 | 6 |

-50-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 1017 | C | GLY | A | 129 | 47.468 | 16.152 | 3.484 | 1.00 | 21.29 | 6 |
| | ATOM | 1018 | O | GLY | A | 129 | 46.782 | 15.601 | 4.321 | 1.00 | 21.30 | 8 |
| | ATOM | 1019 | N | VAL | A | 130 | 47.317 | 16.084 | 2.166 | 1.00 | 21.70 | 7 |
| 5 | ATOM | 1020 | CA | VAL | A | 130 | 46.441 | 15.028 | 1.634 | 1.00 | 21.40 | 6 |
| | ATOM | 1021 | C | VAL | A | 130 | 46.908 | 13.587 | 1.970 | 1.00 | 20.52 | 6 |
| | ATOM | 1022 | O | VAL | A | 130 | 46.140 | 12.807 | 2.542 | 1.00 | 19.78 | 8 |
| | ATOM | 1023 | CB | VAL | A | 130 | 46.256 | 15.179 | 0.107 | 1.00 | 22.23 | 6 |
| | ATOM | 1024 | CG1 | VAL | A | 130 | 45.496 | 13.992 | -0.479 | 1.00 | 22.29 | 6 |
| 10 | ATOM | 1025 | CG2 | VAL | A | 130 | 45.587 | 16.550 | -0.161 | 1.00 | 22.53 | 6 |
| | ATOM | 1026 | N | SER | A | 131 | 48.184 | 13.286 | 1.709 | 1.00 | 22.62 | 7 |
| | ATOM | 1027 | CA | SER | A | 131 | 48.669 | 11.951 | 2.032 | 1.00 | 22.39 | 6 |
| | ATOM | 1028 | C | SER | A | 131 | 48.617 | 11.685 | 3.541 | 1.00 | 20.26 | 6 |
| | ATOM | 1029 | O | SER | A | 131 | 48.328 | 10.545 | 3.924 | 1.00 | 22.14 | 8 |
| 15 | ATOM | 1030 | CB | SER | A | 131 | 50.095 | 11.641 | 1.549 | 1.00 | 22.52 | 6 |
| | ATOM | 1031 | OG | SER | A | 131 | 50.924 | 12.773 | 1.784 | 1.00 | 24.21 | 8 |
| | ATOM | 1032 | N | THR | A | 132 | 48.883 | 12.678 | 4.393 | 1.00 | 17.99 | 7 |
| | ATOM | 1033 | CA | THR | A | 132 | 48.785 | 12.419 | 5.812 | 1.00 | 17.46 | 6 |
| | ATOM | 1034 | C | THR | A | 132 | 47.375 | 12.119 | 6.296 | 1.00 | 17.48 | 6 |
| 20 | ATOM | 1035 | O | THR | A | 132 | 47.180 | 11.104 | 7.013 | 1.00 | 17.25 | 8 |
| | ATOM | 1036 | CB | THR | A | 132 | 49.386 | 13.645 | 6.619 | 1.00 | 17.40 | 6 |
| | ATOM | 1037 | OG1 | THR | A | 132 | 50.726 | 13.812 | 6.145 | 1.00 | 20.91 | 8 |
| | ATOM | 1038 | CG2 | THR | A | 132 | 49.302 | 13.374 | 8.096 | 1.00 | 18.97 | 6 |
| | ATOM | 1039 | N | ILE | A | 133 | 46.378 | 12.918 | 5.840 | 1.00 | 17.51 | 7 |
| 25 | ATOM | 1040 | CA | ILE | A | 133 | 45.048 | 12.635 | 6.366 | 1.00 | 17.42 | 6 |
| | ATOM | 1041 | C | ILE | A | 133 | 44.514 | 11.317 | 5.727 | 1.00 | 17.76 | 6 |
| | ATOM | 1042 | O | ILE | A | 133 | 43.831 | 10.598 | 6.432 | 1.00 | 16.73 | 8 |
| | ATOM | 1043 | CB | ILE | A | 133 | 44.056 | 13.814 | 6.199 | 1.00 | 19.04 | 6 |
| | ATOM | 1044 | CG1 | ILE | A | 133 | 42.772 | 13.574 | 6.991 | 1.00 | 18.12 | 6 |
| 30 | ATOM | 1045 | CG2 | ILE | A | 133 | 43.692 | 14.007 | 4.713 | 1.00 | 19.62 | 6 |
| | ATOM | 1046 | CD1 | ILE | A | 133 | 43.077 | 13.562 | 8.543 | 1.00 | 19.23 | 6 |
| | ATOM | 1047 | N | VAL | A | 134 | 44.834 | 11.013 | 4.468 | 1.00 | 20.06 | 7 |
| | ATOM | 1048 | CA | VAL | A | 134 | 44.318 | 9.805 | 3.843 | 1.00 | 20.66 | 6 |
| | ATOM | 1049 | C | VAL | A | 134 | 44.943 | 8.567 | 4.523 | 1.00 | 16.68 | 6 |
| 35 | ATOM | 1050 | O | VAL | A | 134 | 44.181 | 7.608 | 4.840 | 1.00 | 16.16 | 8 |
| | ATOM | 1051 | CB | VAL | A | 134 | 44.556 | 9.769 | 2.329 | 1.00 | 20.12 | 6 |
| | ATOM | 1052 | CG1 | VAL | A | 134 | 43.968 | 8.529 | 1.685 | 1.00 | 20.31 | 6 |
| | ATOM | 1053 | CG2 | VAL | A | 134 | 43.953 | 11.019 | 1.680 | 1.00 | 21.96 | 6 |
| | ATOM | 1054 | N | SER | A | 135 | 46.232 | 8.622 | 4.793 | 1.00 | 17.42 | 7 |
| 40 | ATOM | 1055 | CA | SER | A | 135 | 46.862 | 7.515 | 5.554 | 1.00 | 18.57 | 6 |
| | ATOM | 1056 | C | SER | A | 135 | 46.167 | 7.337 | 6.870 | 1.00 | 18.10 | 6 |
| | ATOM | 1057 | O | SER | A | 135 | 45.906 | 6.226 | 7.307 | 1.00 | 17.58 | 8 |
| | ATOM | 1058 | CB | SER | A | 135 | 48.367 | 7.725 | 5.776 | 1.00 | 21.85 | 6 |
| | ATOM | 1059 | OG | SER | A | 135 | 49.165 | 7.574 | 4.629 | 1.00 | 26.07 | 8 |
| 45 | ATOM | 1060 | N | LYS | A | 136 | 45.960 | 8.454 | 7.642 | 1.00 | 17.06 | 7 |
| | ATOM | 1061 | CA | LYS | A | 136 | 45.344 | 8.319 | 8.939 | 1.00 | 16.75 | 6 |
| | ATOM | 1062 | C | LYS | A | 136 | 43.943 | 7.726 | 8.855 | 1.00 | 16.59 | 6 |
| | ATOM | 1063 | O | LYS | A | 136 | 43.549 | 6.804 | 9.565 | 1.00 | 17.77 | 8 |
| | ATOM | 1064 | CB | LYS | A | 136 | 45.347 | 9.698 | 9.654 | 1.00 | 17.50 | 6 |
| 50 | ATOM | 1065 | CG | LYS | A | 136 | 44.778 | 9.658 | 11.055 | 1.00 | 17.92 | 6 |
| | ATOM | 1066 | CD | LYS | A | 136 | 45.193 | 10.949 | 11.821 | 1.00 | 18.19 | 6 |
| | ATOM | 1067 | CE | LYS | A | 136 | 44.719 | 10.824 | 13.255 | 1.00 | 20.47 | 6 |
| | ATOM | 1068 | NZ | LYS | A | 136 | 45.341 | 11.921 | 14.099 | 1.00 | 21.74 | 7 |
| | ATOM | 1069 | N | LEU | A | 137 | 43.114 | 8.215 | 7.905 | 1.00 | 16.58 | 7 |
| 55 | ATOM | 1070 | CA | LEU | A | 137 | 41.820 | 7.610 | 7.620 | 1.00 | 16.97 | 6 |
| | ATOM | 1071 | C | LEU | A | 137 | 41.917 | 6.145 | 7.208 | 1.00 | 16.87 | 6 |
| | ATOM | 1072 | O | LEU | A | 137 | 41.086 | 5.366 | 7.671 | 1.00 | 18.31 | 8 |
| | ATOM | 1073 | CB | LEU | A | 137 | 41.186 | 8.426 | 6.450 | 1.00 | 16.26 | 6 |
| | ATOM | 1074 | CG | LEU | A | 137 | 40.680 | 9.774 | 6.970 | 1.00 | 19.05 | 6 |
| 60 | ATOM | 1075 | CD1 | LEU | A | 137 | 40.287 | 10.582 | 5.686 | 1.00 | 19.51 | 6 |
| | ATOM | 1076 | CD2 | LEU | A | 137 | 39.540 | 9.723 | 7.939 | 1.00 | 20.72 | 6 |
| | ATOM | 1077 | N | PHE | A | 138 | 42.967 | 5.788 | 6.451 | 1.00 | 16.58 | 7 |
| | ATOM | 1078 | CA | PHE | A | 138 | 43.010 | 4.341 | 6.127 | 1.00 | 18.39 | 6 |
| | ATOM | 1079 | C | PHE | A | 138 | 43.255 | 3.486 | 7.348 | 1.00 | 18.60 | 6 |
| 65 | ATOM | 1080 | O | PHE | A | 138 | 42.757 | 2.384 | 7.504 | 1.00 | 17.30 | 8 |
| | ATOM | 1081 | CB | PHE | A | 138 | 44.122 | 4.115 | 5.093 | 1.00 | 17.12 | 6 |
| | ATOM | 1082 | CG | PHE | A | 138 | 43.764 | 4.570 | 3.689 | 1.00 | 18.73 | 6 |
| | ATOM | 1083 | CD1 | PHE | A | 138 | 44.806 | 4.543 | 2.766 | 1.00 | 17.88 | 6 |
| | ATOM | 1084 | CD2 | PHE | A | 138 | 42.473 | 4.892 | 3.307 | 1.00 | 18.91 | 6 |
| 70 | ATOM | 1085 | CE1 | PHE | A | 138 | 44.536 | 4.879 | 1.448 | 1.00 | 20.01 | 6 |
| | ATOM | 1086 | CE2 | PHE | A | 138 | 42.230 | 5.257 | 1.997 | 1.00 | 19.56 | 6 |
| | ATOM | 1087 | CZ | PHE | A | 138 | 43.254 | 5.215 | 1.074 | 1.00 | 19.96 | 6 |
| | ATOM | 1088 | N | ASN | A | 139 | 44.082 | 4.007 | 8.264 | 1.00 | 18.42 | 7 |
| | ATOM | 1089 | CA | ASN | A | 139 | 44.379 | 3.252 | 9.498 | 1.00 | 18.84 | 6 |
| | ATOM | 1090 | C | ASN | A | 139 | 43.214 | 3.179 | 10.420 | 1.00 | 18.89 | 6 |

-51-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 1091 | O | ASN | A | 139 | 43.006 | 2.188 | 11.154 | 1.00 | 20.77 | 8 |
| | ATOM | 1092 | CB | ASN | A | 139 | 45.584 | 3.896 | 10.226 | 1.00 | 18.65 | 6 |
| | ATOM | 1093 | CG | ASN | A | 139 | 46.893 | 3.695 | 9.486 | 1.00 | 21.58 | 6 |
| 5 | ATOM | 1094 | OD1 | ASN | A | 139 | 47.077 | 2.678 | 8.835 | 1.00 | 23.27 | 8 |
| | ATOM | 1095 | ND2 | ASN | A | 139 | 47.838 | 4.616 | 9.605 | 1.00 | 23.11 | 7 |
| | ATOM | 1096 | N | LEU | A | 140 | 42.380 | 4.245 | 10.477 | 1.00 | 18.73 | 7 |
| | ATOM | 1097 | CA | LEU | A | 140 | 41.227 | 4.287 | 11.337 | 1.00 | 19.89 | 6 |
| | ATOM | 1098 | C | LEU | A | 140 | 40.035 | 3.500 | 10.798 | 1.00 | 22.66 | 6 |
| 10 | ATOM | 1099 | O | LEU | A | 140 | 39.348 | 2.886 | 11.581 | 1.00 | 23.40 | 8 |
| | ATOM | 1100 | CB | LEU | A | 140 | 40.725 | 5.736 | 11.530 | 1.00 | 19.74 | 6 |
| | ATOM | 1101 | CG | LEU | A | 140 | 41.667 | 6.734 | 12.211 | 1.00 | 20.69 | 6 |
| | ATOM | 1102 | CD1 | LEU | A | 140 | 41.159 | 8.189 | 12.222 | 1.00 | 20.47 | 6 |
| | ATOM | 1103 | CD2 | LEU | A | 140 | 41.923 | 6.357 | 13.687 | 1.00 | 21.82 | 6 |
| 15 | ATOM | 1104 | N | VAL | A | 141 | 39.777 | 3.644 | 9.493 | 1.00 | 21.89 | 7 |
| | ATOM | 1105 | CA | VAL | A | 141 | 38.625 | 2.951 | 8.912 | 1.00 | 18.58 | 6 |
| | ATOM | 1106 | C | VAL | A | 141 | 38.930 | 1.566 | 8.477 | 1.00 | 18.27 | 6 |
| | ATOM | 1107 | O | VAL | A | 141 | 37.992 | 0.726 | 8.348 | 1.00 | 21.83 | 8 |
| | ATOM | 1108 | CB | VAL | A | 141 | 38.121 | 3.897 | 7.749 | 1.00 | 17.89 | 6 |
| 20 | ATOM | 1109 | CG1 | VAL | A | 141 | 37.004 | 3.204 | 6.948 | 1.00 | 19.45 | 6 |
| | ATOM | 1110 | CG2 | VAL | A | 141 | 37.684 | 5.229 | 8.360 | 1.00 | 19.31 | 6 |
| | ATOM | 1111 | N | GLN | A | 142 | 40.157 | 1.207 | 8.147 | 1.00 | 19.32 | 7 |
| | ATOM | 1112 | CA | GLN | A | 142 | 40.614 | -0.046 | 7.611 | 1.00 | 22.31 | 6 |
| | ATOM | 1113 | C | GLN | A | 142 | 39.731 | -0.535 | 6.460 | 1.00 | 19.60 | 6 |
| 25 | ATOM | 1114 | O | GLN | A | 142 | 39.182 | -1.647 | 6.518 | 1.00 | 20.68 | 8 |
| | ATOM | 1115 | CB | GLN | A | 142 | 40.661 | -1.162 | 8.674 | 1.00 | 23.95 | 6 |
| | ATOM | 1116 | CG | GLN | A | 142 | 41.594 | -0.685 | 9.829 | 1.00 | 28.73 | 6 |
| | ATOM | 1117 | CD | GLN | A | 142 | 41.536 | -1.705 | 10.951 | 1.00 | 34.39 | 6 |
| | ATOM | 1118 | OE1 | GLN | A | 142 | 42.491 | -2.469 | 11.021 | 1.00 | 39.24 | 8 |
| 30 | ATOM | 1119 | NE2 | GLN | A | 142 | 40.502 | -1.784 | 11.754 | 1.00 | 35.26 | 7 |
| | ATOM | 1120 | N | PRO | A | 143 | 39.558 | 0.297 | 5.442 | 1.00 | 18.88 | 7 |
| | ATOM | 1121 | CA | PRO | A | 143 | 38.717 | -0.119 | 4.346 | 1.00 | 18.57 | 6 |
| | ATOM | 1122 | C | PRO | A | 143 | 39.398 | -1.140 | 3.497 | 1.00 | 19.27 | 6 |
| | ATOM | 1123 | O | PRO | A | 143 | 40.627 | -1.225 | 3.382 | 1.00 | 21.22 | 8 |
| 35 | ATOM | 1124 | CB | PRO | A | 143 | 38.538 | 1.179 | 3.558 | 1.00 | 17.81 | 6 |
| | ATOM | 1125 | CG | PRO | A | 143 | 39.829 | 1.905 | 3.755 | 1.00 | 17.73 | 6 |
| | ATOM | 1126 | CD | PRO | A | 143 | 40.201 | 1.627 | 5.230 | 1.00 | 17.54 | 6 |
| | ATOM | 1127 | N | ASP | A | 144 | 38.648 | -1.982 | 2.768 | 1.00 | 17.55 | 7 |
| | ATOM | 1128 | CA | ASP | A | 144 | 39.097 | -2.852 | 1.720 | 1.00 | 20.28 | 6 |
| 40 | ATOM | 1129 | C | ASP | A | 144 | 39.283 | -2.125 | 0.399 | 1.00 | 19.25 | 6 |
| | ATOM | 1130 | O | ASP | A | 144 | 40.083 | -2.459 | -0.481 | 1.00 | 20.98 | 8 |
| | ATOM | 1131 | CB | ASP | A | 144 | 38.033 | -3.936 | 1.546 | 1.00 | 20.76 | 6 |
| | ATOM | 1132 | CG | ASP | A | 144 | 37.957 | -4.815 | 2.798 | 1.00 | 26.72 | 6 |
| | ATOM | 1133 | OD1 | ASP | A | 144 | 36.961 | -4.629 | 3.528 | 1.00 | 28.28 | 8 |
| 45 | ATOM | 1134 | OD2 | ASP | A | 144 | 38.895 | -5.587 | 3.031 | 1.00 | 31.50 | 8 |
| | ATOM | 1135 | N | ILE | A | 145 | 38.477 | -1.081 | 0.131 | 1.00 | 17.25 | 7 |
| | ATOM | 1136 | CA | ILE | A | 145 | 38.375 | -0.260 | -1.035 | 1.00 | 18.60 | 6 |
| | ATOM | 1137 | C | ILE | A | 145 | 38.239 | 1.190 | -0.687 | 1.00 | 18.09 | 6 |
| | ATOM | 1138 | O | ILE | A | 145 | 37.607 | 1.491 | 0.327 | 1.00 | 18.47 | 8 |
| 50 | ATOM | 1139 | CB | ILE | A | 145 | 37.081 | -0.719 | -1.802 | 1.00 | 22.13 | 6 |
| | ATOM | 1140 | CG1 | ILE | A | 145 | 37.350 | -2.164 | -2.291 | 1.00 | 26.63 | 6 |
| | ATOM | 1141 | CG2 | ILE | A | 145 | 36.613 | 0.193 | -2.934 | 1.00 | 28.58 | 6 |
| | ATOM | 1142 | CD1 | ILE | A | 145 | 35.987 | -2.820 | -2.537 | 1.00 | 33.01 | 6 |
| | ATOM | 1143 | N | ALA | A | 146 | 38.745 | 2.119 | -1.471 | 1.00 | 18.54 | 7 |
| 55 | ATOM | 1144 | CA | ALA | A | 146 | 38.555 | 3.525 | -1.287 | 1.00 | 17.65 | 6 |
| | ATOM | 1145 | C | ALA | A | 146 | 38.386 | 4.174 | -2.669 | 1.00 | 18.82 | 6 |
| | ATOM | 1146 | O | ALA | A | 146 | 39.158 | 3.831 | -3.590 | 1.00 | 20.86 | 8 |
| | ATOM | 1147 | CB | ALA | A | 146 | 39.754 | 4.169 | -0.561 | 1.00 | 17.02 | 6 |
| | ATOM | 1148 | N | CYS | A | 147 | 37.421 | 5.032 | -2.758 | 1.00 | 17.39 | 7 |
| 60 | ATOM | 1149 | CA | CYS | A | 147 | 37.059 | 5.669 | -4.042 | 1.00 | 19.79 | 6 |
| | ATOM | 1150 | C | CYS | A | 147 | 37.462 | 7.132 | -4.108 | 1.00 | 20.20 | 6 |
| | ATOM | 1151 | O | CYS | A | 147 | 37.292 | 7.934 | -3.181 | 1.00 | 20.69 | 8 |
| | ATOM | 1152 | CB | CYS | A | 147 | 35.534 | 5.576 | -4.235 | 1.00 | 21.84 | 6 |
| | ATOM | 1153 | SG | CYS | A | 147 | 34.881 | 3.895 | -4.275 | 1.00 | 25.91 | 16 |
| 65 | ATOM | 1154 | N | PHE | A | 148 | 38.073 | 7.481 | -5.256 | 1.00 | 20.78 | 7 |
| | ATOM | 1155 | CA | PHE | A | 148 | 38.521 | 8.824 | -5.534 | 1.00 | 20.56 | 6 |
| | ATOM | 1156 | C | PHE | A | 148 | 38.105 | 9.201 | -6.955 | 1.00 | 20.31 | 6 |
| | ATOM | 1157 | O | PHE | A | 148 | 38.047 | 8.291 | -7.790 | 1.00 | 21.33 | 8 |
| | ATOM | 1158 | CB | PHE | A | 148 | 40.044 | 8.856 | -5.392 | 1.00 | 19.98 | 6 |
| 70 | ATOM | 1159 | CG | PHE | A | 148 | 40.527 | 8.697 | -3.964 | 1.00 | 21.76 | 6 |
| | ATOM | 1160 | CD1 | PHE | A | 148 | 40.803 | 7.418 | -3.472 | 1.00 | 21.62 | 6 |
| | ATOM | 1161 | CD2 | PHE | A | 148 | 40.682 | 9.781 | -3.137 | 1.00 | 24.08 | 6 |
| | ATOM | 1162 | CE1 | PHE | A | 148 | 41.217 | 7.237 | -2.164 | 1.00 | 21.64 | 6 |
| | ATOM | 1163 | CE2 | PHE | A | 148 | 41.150 | 9.580 | -1.833 | 1.00 | 22.23 | 6 |
| | ATOM | 1164 | CZ | PHE | A | 148 | 41.384 | 8.321 | -1.337 | 1.00 | 21.48 | 6 |

-52-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1165 | N | GLY | A | 149 | 37.874 | 10.485 | -7.215 | 1.00 | 19.66 | 7 |
| | ATOM | 1166 | CA | GLY | A | 149 | 37.457 | 10.782 | -8.630 | 1.00 | 19.28 | 6 |
| | ATOM | 1167 | C | GLY | A | 149 | 38.663 | 10.981 | -9.537 | 1.00 | 21.16 | 6 |
| 5 | ATOM | 1168 | O | GLY | A | 149 | 39.696 | 11.548 | -9.117 | 1.00 | 25.03 | 8 |
| | ATOM | 1169 | N | GLU | A | 150 | 38.524 | 10.707 | -10.848 | 1.00 | 21.70 | 7 |
| | ATOM | 1170 | CA | GLU | A | 150 | 39.588 | 10.939 | -11.809 | 1.00 | 25.98 | 6 |
| | ATOM | 1171 | C | GLU | A | 150 | 39.777 | 12.386 | -12.160 | 1.00 | 25.10 | 6 |
| | ATOM | 1172 | O | GLU | A | 150 | 40.841 | 12.764 | -12.668 | 1.00 | 26.55 | 8 |
| 10 | ATOM | 1173 | CB | GLU | A | 150 | 39.316 | 10.178 | -13.146 | 1.00 | 28.34 | 6 |
| | ATOM | 1174 | CG | GLU | A | 150 | 39.447 | 8.683 | -12.924 | 1.00 | 30.38 | 6 |
| | ATOM | 1175 | CD | GLU | A | 150 | 39.464 | 7.923 | -14.241 | 1.00 | 36.75 | 6 |
| | ATOM | 1176 | OE1 | GLU | A | 150 | 39.222 | 8.536 | -15.309 | 1.00 | 39.43 | 8 |
| | ATOM | 1177 | OE2 | GLU | A | 150 | 39.770 | 6.715 | -14.171 | 1.00 | 39.37 | 8 |
| 15 | ATOM | 1178 | N | LYS | A | 151 | 38.795 | 13.240 | -11.874 | 1.00 | 25.17 | 7 |
| | ATOM | 1179 | CA | LYS | A | 151 | 38.970 | 14.660 | -12.162 | 1.00 | 28.17 | 6 |
| | ATOM | 1180 | C | LYS | A | 151 | 40.159 | 15.229 | -11.400 | 1.00 | 29.47 | 6 |
| | ATOM | 1181 | O | LYS | A | 151 | 40.955 | 16.017 | -11.930 | 1.00 | 29.69 | 8 |
| | ATOM | 1182 | CB | LYS | A | 151 | 37.710 | 15.423 | -11.787 | 1.00 | 30.49 | 6 |
| 20 | ATOM | 1183 | CG | LYS | A | 151 | 37.865 | 16.877 | -12.255 | 1.00 | 34.63 | 6 |
| | ATOM | 1184 | CD | LYS | A | 151 | 37.021 | 17.827 | -11.434 | 1.00 | 40.81 | 6 |
| | ATOM | 1185 | CE | LYS | A | 151 | 37.161 | 19.249 | -12.007 | 1.00 | 42.71 | 6 |
| | ATOM | 1186 | NZ | LYS | A | 151 | 35.905 | 20.032 | -11.825 | 1.00 | 46.87 | 7 |
| | ATOM | 1187 | N | ASP | A | 152 | 40.274 | 14.877 | -10.114 | 1.00 | 26.84 | 7 |
| 25 | ATOM | 1188 | CA | ASP | A | 152 | 41.456 | 15.268 | -9.322 | 1.00 | 26.83 | 6 |
| | ATOM | 1189 | C | ASP | A | 152 | 42.545 | 14.241 | -9.529 | 1.00 | 26.30 | 6 |
| | ATOM | 1190 | O | ASP | A | 152 | 42.933 | 13.366 | -8.715 | 1.00 | 24.28 | 8 |
| | ATOM | 1191 | CB | ASP | A | 152 | 41.078 | 15.419 | -7.846 | 1.00 | 29.39 | 6 |
| | ATOM | 1192 | N | PHE | A | 153 | 43.137 | 14.340 | -10.746 | 1.00 | 24.76 | 7 |
| 30 | ATOM | 1193 | CA | PHE | A | 153 | 44.063 | 13.342 | -11.241 | 1.00 | 24.28 | 6 |
| | ATOM | 1194 | C | PHE | A | 153 | 45.350 | 13.353 | -10.435 | 1.00 | 24.40 | 6 |
| | ATOM | 1195 | O | PHE | A | 153 | 45.891 | 12.270 | -10.274 | 1.00 | 24.91 | 8 |
| | ATOM | 1196 | CB | PHE | A | 153 | 44.385 | 13.509 | -12.748 | 1.00 | 26.30 | 6 |
| | ATOM | 1197 | CG | PHE | A | 153 | 45.137 | 14.809 | -12.939 | 1.00 | 29.67 | 6 |
| 35 | ATOM | 1198 | CD1 | PHE | A | 153 | 46.517 | 14.828 | -13.025 | 1.00 | 30.48 | 6 |
| | ATOM | 1199 | CD2 | PHE | A | 153 | 44.443 | 16.015 | -13.033 | 1.00 | 32.69 | 6 |
| | ATOM | 1200 | CE1 | PHE | A | 153 | 47.203 | 16.017 | -13.147 | 1.00 | 31.59 | 6 |
| | ATOM | 1201 | CE2 | PHE | A | 153 | 45.124 | 17.212 | -13.186 | 1.00 | 33.09 | 6 |
| | ATOM | 1202 | CZ | PHE | A | 153 | 46.511 | 17.215 | -13.241 | 1.00 | 34.20 | 6 |
| 40 | ATOM | 1203 | N | GLN | A | 154 | 45.781 | 14.510 | -9.931 | 1.00 | 25.98 | 7 |
| | ATOM | 1204 | CA | GLN | A | 154 | 47.028 | 14.521 | -9.174 | 1.00 | 22.85 | 6 |
| | ATOM | 1205 | C | GLN | A | 154 | 46.851 | 13.825 | -7.837 | 1.00 | 22.38 | 6 |
| | ATOM | 1206 | O | GLN | A | 154 | 47.695 | 13.032 | -7.413 | 1.00 | 22.53 | 8 |
| | ATOM | 1207 | CB | GLN | A | 154 | 47.542 | 15.952 | -8.933 | 1.00 | 24.08 | 6 |
| 45 | ATOM | 1208 | CG | GLN | A | 154 | 48.929 | 15.967 | -8.287 | 1.00 | 26.39 | 6 |
| | ATOM | 1209 | CD | GLN | A | 154 | 49.688 | 17.287 | -8.508 | 1.00 | 28.37 | 6 |
| | ATOM | 1210 | OE1 | GLN | A | 154 | 49.098 | 18.244 | -8.993 | 1.00 | 28.49 | 8 |
| | ATOM | 1211 | NE2 | GLN | A | 154 | 50.978 | 17.318 | -8.158 | 1.00 | 26.87 | 7 |
| | ATOM | 1212 | N | GLN | A | 155 | 45.747 | 14.096 | -7.174 | 1.00 | 21.22 | 7 |
| 50 | ATOM | 1213 | CA | GLN | A | 155 | 45.470 | 13.411 | -5.896 | 1.00 | 21.76 | 6 |
| | ATOM | 1214 | C | GLN | A | 155 | 45.362 | 11.902 | -6.092 | 1.00 | 21.39 | 6 |
| | ATOM | 1215 | O | GLN | A | 155 | 45.852 | 11.100 | -5.289 | 1.00 | 20.96 | 8 |
| | ATOM | 1216 | CB | GLN | A | 155 | 44.157 | 13.885 | -5.251 | 1.00 | 23.33 | 6 |
| | ATOM | 1217 | CG | GLN | A | 155 | 44.285 | 15.020 | -4.241 | 0.50 | 22.16 | 6 |
| | ATOM | 1218 | CD | GLN | A | 155 | 43.185 | 14.991 | -3.184 | 0.50 | 22.84 | 6 |
| 55 | ATOM | 1219 | OE1 | GLN | A | 155 | 42.574 | 13.952 | -2.872 | 0.50 | 25.23 | 8 |
| | ATOM | 1220 | NE2 | GLN | A | 155 | 42.921 | 16.140 | -2.600 | 0.50 | 20.85 | 7 |
| | ATOM | 1221 | N | LEU | A | 156 | 44.752 | 11.455 | -7.214 | 1.00 | 20.25 | 7 |
| | ATOM | 1222 | CA | LEU | A | 156 | 44.592 | 10.045 | -7.465 | 1.00 | 18.93 | 6 |
| 60 | ATOM | 1223 | C | LEU | A | 156 | 45.938 | 9.367 | -7.681 | 1.00 | 20.91 | 6 |
| | ATOM | 1224 | O | LEU | A | 156 | 46.240 | 8.334 | -7.081 | 1.00 | 20.99 | 8 |
| | ATOM | 1225 | CB | LEU | A | 156 | 43.684 | 9.840 | -8.695 | 1.00 | 20.06 | 6 |
| | ATOM | 1226 | CG | LEU | A | 156 | 43.409 | 8.396 | -9.060 | 1.00 | 21.79 | 6 |
| | ATOM | 1227 | CD1 | LEU | A | 156 | 42.773 | 7.624 | -7.893 | 1.00 | 20.19 | 6 |
| | ATOM | 1228 | CD2 | LEU | A | 156 | 42.493 | 8.367 | -10.300 | 1.00 | 23.41 | 6 |
| 65 | ATOM | 1229 | N | ALA | A | 157 | 46.790 | 9.991 | -8.498 | 1.00 | 21.27 | 7 |
| | ATOM | 1230 | CA | ALA | A | 157 | 48.139 | 9.424 | -8.654 | 1.00 | 20.85 | 6 |
| | ATOM | 1231 | C | ALA | A | 157 | 48.896 | 9.402 | -7.339 | 1.00 | 22.15 | 6 |
| | ATOM | 1232 | O | ALA | A | 157 | 49.617 | 8.451 | -7.039 | 1.00 | 23.09 | 8 |
| | ATOM | 1233 | CB | ALA | A | 157 | 48.919 | 10.292 | -9.658 | 1.00 | 21.65 | 6 |
| 70 | ATOM | 1234 | N | LEU | A | 158 | 48.771 | 10.447 | -6.537 | 1.00 | 21.63 | 7 |
| | ATOM | 1235 | CA | LEU | A | 158 | 49.507 | 10.508 | -5.235 | 1.00 | 20.79 | 6 |
| | ATOM | 1236 | C | LEU | A | 158 | 49.117 | 9.373 | -4.311 | 1.00 | 22.51 | 6 |
| | ATOM | 1237 | O | LEU | A | 158 | 49.950 | 8.663 | -3.702 | 1.00 | 22.35 | 8 |
| | ATOM | 1238 | CB | LEU | A | 158 | 49.227 | 11.847 | -4.583 | 1.00 | 23.18 | 6 |

-53-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|----|
| | ATOM | 1239 | CG | LEU | A | 158 | 49.828 | 12.175 | -3.211 | 1.00 | 25.19 | 6 |
| | ATOM | 1240 | CD1 | LEU | A | 158 | 51.099 | 12.952 | -3.381 | 1.00 | 28.19 | 6 |
| | ATOM | 1241 | CD2 | LEU | A | 158 | 48.782 | 12.989 | -2.433 | 1.00 | 26.28 | 6 |
| | ATOM | 1242 | N | ILE | A | 159 | 47.765 | 9.231 | -4.212 | 1.00 | 18.01 | 7 |
| 5 | ATOM | 1243 | CA | ILE | A | 159 | 47.322 | 8.127 | -3.317 | 1.00 | 19.99 | 6 |
| | ATOM | 1244 | C | ILE | A | 159 | 47.680 | 6.760 | -3.864 | 1.00 | 18.66 | 6 |
| | ATOM | 1245 | O | ILE | A | 159 | 48.038 | 5.871 | -3.083 | 1.00 | 19.24 | 8 |
| | ATOM | 1246 | CB | ILE | A | 159 | 45.805 | 8.275 | -3.083 | 1.00 | 23.08 | 6 |
| 10 | ATOM | 1247 | CG1 | ILE | A | 159 | 45.455 | 9.626 | -2.443 | 1.00 | 21.73 | 6 |
| | ATOM | 1248 | CG2 | ILE | A | 159 | 45.232 | 7.181 | -2.187 | 1.00 | 23.20 | 6 |
| | ATOM | 1249 | CD1 | ILE | A | 159 | 46.056 | 9.774 | -1.063 | 1.00 | 27.28 | 6 |
| | ATOM | 1250 | N | ARG | A | 160 | 47.514 | 6.493 | -5.148 | 1.00 | 20.78 | 7 |
| | ATOM | 1251 | CA | ARG | A | 160 | 47.956 | 5.202 | -5.694 | 1.00 | 20.24 | 6 |
| | ATOM | 1252 | C | ARG | A | 160 | 49.422 | 4.914 | -5.397 | 1.00 | 21.57 | 6 |
| 15 | ATOM | 1253 | O | ARG | A | 160 | 49.738 | 3.802 | -4.971 | 1.00 | 19.80 | 8 |
| | ATOM | 1254 | CB | ARG | A | 160 | 47.708 | 5.074 | -7.218 | 1.00 | 21.86 | 6 |
| | ATOM | 1255 | CG | ARG | A | 160 | 46.192 | 5.007 | -7.567 | 1.00 | 21.60 | 6 |
| | ATOM | 1256 | CD | ARG | A | 160 | 46.195 | 4.575 | -9.066 | 1.00 | 25.76 | 6 |
| 20 | ATOM | 1257 | NE | ARG | A | 160 | 44.867 | 4.625 | -9.678 | 1.00 | 29.84 | 7 |
| | ATOM | 1258 | CZ | ARG | A | 160 | 43.905 | 3.713 | -9.455 | 1.00 | 32.53 | 6 |
| | ATOM | 1259 | NH1 | ARG | A | 160 | 44.040 | 2.653 | -8.651 | 1.00 | 32.58 | 7 |
| | ATOM | 1260 | NH2 | ARG | A | 160 | 42.788 | 3.911 | -10.168 | 1.00 | 34.80 | 7 |
| | ATOM | 1261 | N | LYS | A | 161 | 50.322 | 5.905 | -5.460 | 1.00 | 20.74 | 7 |
| 25 | ATOM | 1262 | CA | LYS | A | 161 | 51.733 | 5.714 | -5.164 | 1.00 | 19.39 | 6 |
| | ATOM | 1263 | C | LYS | A | 161 | 51.925 | 5.506 | -3.674 | 1.00 | 19.31 | 6 |
| | ATOM | 1264 | O | LYS | A | 161 | 52.628 | 4.596 | -3.191 | 1.00 | 22.15 | 8 |
| | ATOM | 1265 | CB | LYS | A | 161 | 52.523 | 6.929 | -5.649 | 1.00 | 21.10 | 6 |
| | ATOM | 1266 | CG | LYS | A | 161 | 54.009 | 6.900 | -5.202 | 1.00 | 24.79 | 6 |
| 30 | ATOM | 1267 | CD | LYS | A | 161 | 54.612 | 5.615 | -5.820 | 1.00 | 28.31 | 6 |
| | ATOM | 1268 | CE | LYS | A | 161 | 56.100 | 5.758 | -6.162 | 1.00 | 31.56 | 6 |
| | ATOM | 1269 | NZ | LYS | A | 161 | 56.913 | 6.424 | -5.128 | 1.00 | 26.44 | 7 |
| | ATOM | 1270 | N | MET | A | 162 | 51.191 | 6.312 | -2.834 | 1.00 | 20.30 | 7 |
| | ATOM | 1271 | CA | MET | A | 162 | 51.287 | 6.115 | -1.383 | 1.00 | 18.85 | 6 |
| 35 | ATOM | 1272 | C | MET | A | 162 | 50.851 | 4.750 | -0.908 | 1.00 | 21.35 | 6 |
| | ATOM | 1273 | O | MET | A | 162 | 51.504 | 4.085 | -0.089 | 1.00 | 20.93 | 8 |
| | ATOM | 1274 | CB | MET | A | 162 | 50.412 | 7.231 | -0.702 | 1.00 | 21.14 | 6 |
| | ATOM | 1275 | CG | MET | A | 162 | 50.512 | 7.132 | 0.818 | 1.00 | 21.47 | 6 |
| | ATOM | 1276 | SD | MET | A | 162 | 49.291 | 8.186 | 1.642 | 1.00 | 23.59 | 16 |
| 40 | ATOM | 1277 | CE | MET | A | 162 | 47.948 | 6.994 | 1.780 | 1.00 | 27.52 | 6 |
| | ATOM | 1278 | N | VAL | A | 163 | 49.808 | 4.217 | -1.577 | 1.00 | 19.66 | 7 |
| | ATOM | 1279 | CA | VAL | A | 163 | 49.304 | 2.897 | -1.214 | 1.00 | 20.50 | 6 |
| | ATOM | 1280 | C | VAL | A | 163 | 50.289 | 1.806 | -1.612 | 1.00 | 19.37 | 6 |
| | ATOM | 1281 | O | VAL | A | 163 | 50.554 | 0.867 | -0.837 | 1.00 | 20.07 | 8 |
| 45 | ATOM | 1282 | CB | VAL | A | 163 | 47.914 | 2.672 | -1.873 | 1.00 | 21.79 | 6 |
| | ATOM | 1283 | CG1 | VAL | A | 163 | 47.540 | 1.204 | -1.894 | 1.00 | 22.15 | 6 |
| | ATOM | 1284 | CG2 | VAL | A | 163 | 46.897 | 3.536 | -1.100 | 1.00 | 22.77 | 6 |
| | ATOM | 1285 | N | ALA | A | 164 | 50.784 | 1.931 | -2.837 | 1.00 | 21.03 | 7 |
| | ATOM | 1286 | CA | ALA | A | 164 | 51.773 | 0.937 | -3.276 | 1.00 | 22.98 | 6 |
| 50 | ATOM | 1287 | C | ALA | A | 164 | 53.006 | 0.925 | -2.380 | 1.00 | 23.44 | 6 |
| | ATOM | 1288 | O | ALA | A | 164 | 53.478 | -0.126 | -1.927 | 1.00 | 23.96 | 8 |
| | ATOM | 1289 | CB | ALA | A | 164 | 52.136 | 1.263 | -4.719 | 1.00 | 23.95 | 6 |
| | ATOM | 1290 | N | ASP | A | 165 | 53.552 | 2.121 | -2.154 | 1.00 | 21.54 | 7 |
| | ATOM | 1291 | CA | ASP | A | 165 | 54.788 | 2.231 | -1.387 | 1.00 | 23.74 | 6 |
| 55 | ATOM | 1292 | C | ASP | A | 165 | 54.639 | 1.784 | 0.052 | 1.00 | 24.26 | 6 |
| | ATOM | 1293 | O | ASP | A | 165 | 55.440 | 1.000 | 0.544 | 1.00 | 24.84 | 8 |
| | ATOM | 1294 | CB | ASP | A | 165 | 55.321 | 3.664 | -1.384 | 1.00 | 22.61 | 6 |
| | ATOM | 1295 | CG | ASP | A | 165 | 55.980 | 4.130 | -2.662 | 1.00 | 24.69 | 6 |
| | ATOM | 1296 | OD1 | ASP | A | 165 | 56.269 | 3.286 | -3.531 | 1.00 | 24.19 | 8 |
| 60 | ATOM | 1297 | OD2 | ASP | A | 165 | 56.220 | 5.356 | -2.781 | 1.00 | 24.88 | 8 |
| | ATOM | 1298 | N | MET | A | 166 | 53.590 | 2.288 | 0.725 | 1.00 | 21.43 | 7 |
| | ATOM | 1299 | CA | MET | A | 166 | 53.378 | 2.007 | 2.157 | 1.00 | 20.10 | 6 |
| | ATOM | 1300 | C | MET | A | 166 | 52.785 | 0.652 | 2.486 | 1.00 | 21.04 | 6 |
| | ATOM | 1301 | O | MET | A | 166 | 52.605 | 0.347 | 3.671 | 1.00 | 21.28 | 8 |
| 65 | ATOM | 1302 | CB | MET | A | 166 | 52.540 | 3.142 | 2.751 | 1.00 | 20.75 | 6 |
| | ATOM | 1303 | CG | MET | A | 166 | 53.288 | 4.458 | 2.868 | 1.00 | 22.14 | 6 |
| | ATOM | 1304 | SD | MET | A | 166 | 55.034 | 4.259 | 3.242 | 1.00 | 26.84 | 16 |
| | ATOM | 1305 | CE | MET | A | 166 | 54.959 | 3.835 | 4.983 | 1.00 | 27.47 | 6 |
| | ATOM | 1306 | N | GLY | A | 167 | 52.458 | -0.170 | 1.510 | 1.00 | 20.03 | 7 |
| 70 | ATOM | 1307 | CA | GLY | A | 167 | 51.975 | -1.522 | 1.790 | 1.00 | 22.00 | 6 |
| | ATOM | 1308 | C | GLY | A | 167 | 50.526 | -1.606 | 2.218 | 1.00 | 20.49 | 6 |
| | ATOM | 1309 | O | GLY | A | 167 | 50.190 | -2.660 | 2.782 | 1.00 | 24.46 | 8 |
| | ATOM | 1310 | N | PHE | A | 168 | 49.685 | -0.585 | 2.002 | 1.00 | 21.54 | 7 |
| | ATOM | 1311 | CA | PHE | A | 168 | 48.287 | -0.824 | 2.403 | 1.00 | 20.47 | 6 |
| | ATOM | 1312 | C | PHE | A | 168 | 47.645 | -1.917 | 1.546 | 1.00 | 19.05 | 6 |

-54-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1313 | O | PHE | A | 168 | 47.704 | -1.739 | 0.320 | 1.00 | 20.71 | 8 |
| | ATOM | 1314 | CB | PHE | A | 168 | 47.563 | 0.509 | 2.296 | 1.00 | 21.24 | 6 |
| | ATOM | 1315 | CG | PHE | A | 168 | 47.788 | 1.632 | 3.277 | 1.00 | 20.78 | 6 |
| 5 | ATOM | 1316 | CD1 | PHE | A | 168 | 48.548 | 2.751 | 2.932 | 1.00 | 22.23 | 6 |
| | ATOM | 1317 | CD2 | PHE | A | 168 | 47.186 | 1.509 | 4.509 | 1.00 | 21.78 | 6 |
| | ATOM | 1318 | CE1 | PHE | A | 168 | 48.736 | 3.747 | 3.913 | 1.00 | 20.66 | 6 |
| | ATOM | 1319 | CE2 | PHE | A | 168 | 47.353 | 2.544 | 5.432 | 1.00 | 19.66 | 6 |
| | ATOM | 1320 | CZ | PHE | A | 168 | 48.085 | 3.665 | 5.136 | 1.00 | 20.15 | 6 |
| 10 | ATOM | 1321 | N | ASP | A | 169 | 46.769 | -2.693 | 2.126 | 1.00 | 22.42 | 7 |
| | ATOM | 1322 | CA | ASP | A | 169 | 46.084 | -3.767 | 1.356 | 1.00 | 22.89 | 6 |
| | ATOM | 1323 | C | ASP | A | 169 | 44.743 | -3.167 | 0.938 | 1.00 | 23.53 | 6 |
| | ATOM | 1324 | O | ASP | A | 169 | 43.705 | -3.617 | 1.427 | 1.00 | 23.13 | 8 |
| | ATOM | 1325 | CB | ASP | A | 169 | 45.975 | -5.057 | 2.147 | 1.00 | 28.05 | 6 |
| 15 | ATOM | 1326 | CG | ASP | A | 169 | 45.399 | -6.229 | 1.376 | 1.00 | 32.61 | 6 |
| | ATOM | 1327 | OD1 | ASP | A | 169 | 45.492 | -6.192 | 0.129 | 1.00 | 35.09 | 8 |
| | ATOM | 1328 | OD2 | ASP | A | 169 | 44.838 | -7.159 | 1.975 | 1.00 | 37.69 | 8 |
| | ATOM | 1329 | N | ILE | A | 170 | 44.751 | -2.104 | 0.146 | 1.00 | 21.02 | 7 |
| | ATOM | 1330 | CA | ILE | A | 170 | 43.499 | -1.409 | -0.181 | 1.00 | 21.69 | 6 |
| 20 | ATOM | 1331 | C | ILE | A | 170 | 43.372 | -1.265 | -1.677 | 1.00 | 21.49 | 6 |
| | ATOM | 1332 | O | ILE | A | 170 | 44.334 | -0.773 | -2.304 | 1.00 | 22.63 | 8 |
| | ATOM | 1333 | CB | ILE | A | 170 | 43.443 | -0.013 | 0.493 | 1.00 | 21.71 | 6 |
| | ATOM | 1334 | CG1 | ILE | A | 170 | 43.459 | -0.124 | 2.030 | 1.00 | 21.39 | 6 |
| | ATOM | 1335 | CG2 | ILE | A | 170 | 42.221 | 0.770 | 0.037 | 1.00 | 22.28 | 6 |
| 25 | ATOM | 1336 | CD1 | ILE | A | 170 | 43.745 | 1.240 | 2.694 | 1.00 | 23.40 | 6 |
| | ATOM | 1337 | N | GLU | A | 171 | 42.206 | -1.583 | -2.244 | 1.00 | 22.35 | 7 |
| | ATOM | 1338 | CA | GLU | A | 171 | 41.960 | -1.346 | -3.656 | 1.00 | 22.51 | 6 |
| | ATOM | 1339 | C | GLU | A | 171 | 41.609 | 0.133 | -3.871 | 1.00 | 22.05 | 6 |
| | ATOM | 1340 | O | GLU | A | 171 | 40.625 | 0.577 | -3.278 | 1.00 | 20.97 | 8 |
| 30 | ATOM | 1341 | CB | GLU | A | 171 | 40.841 | -2.288 | -4.152 | 1.00 | 21.82 | 6 |
| | ATOM | 1342 | CG | GLU | A | 171 | 40.514 | -1.978 | -5.601 | 1.00 | 28.71 | 6 |
| | ATOM | 1343 | CD | GLU | A | 171 | 39.364 | -2.857 | -6.098 | 1.00 | 34.21 | 6 |
| | ATOM | 1344 | OE1 | GLU | A | 171 | 38.911 | -3.740 | -5.361 | 1.00 | 36.00 | 8 |
| | ATOM | 1345 | OE2 | GLU | A | 171 | 38.953 | -2.650 | -7.272 | 1.00 | 38.31 | 8 |
| 35 | ATOM | 1346 | N | ILE | A | 172 | 42.352 | 0.886 | -4.680 | 1.00 | 20.37 | 7 |
| | ATOM | 1347 | CA | ILE | A | 172 | 42.017 | 2.294 | -4.940 | 1.00 | 19.10 | 6 |
| | ATOM | 1348 | C | ILE | A | 172 | 41.196 | 2.347 | -6.217 | 1.00 | 23.26 | 6 |
| | ATOM | 1349 | O | ILE | A | 172 | 41.716 | 1.875 | -7.239 | 1.00 | 26.08 | 8 |
| | ATOM | 1350 | CB | ILE | A | 172 | 43.306 | 3.159 | -5.019 | 1.00 | 22.26 | 6 |
| 40 | ATOM | 1351 | CG1 | ILE | A | 172 | 44.060 | 2.969 | -3.686 | 1.00 | 21.42 | 6 |
| | ATOM | 1352 | CG2 | ILE | A | 172 | 42.975 | 4.587 | -5.345 | 1.00 | 23.49 | 6 |
| | ATOM | 1353 | CD1 | ILE | A | 172 | 43.283 | 3.498 | -2.483 | 1.00 | 22.09 | 6 |
| | ATOM | 1354 | N | VAL | A | 173 | 39.937 | 2.751 | -6.114 | 1.00 | 20.87 | 7 |
| | ATOM | 1355 | CA | VAL | A | 173 | 39.045 | 2.789 | -7.278 | 1.00 | 23.09 | 6 |
| 45 | ATOM | 1356 | C | VAL | A | 173 | 39.073 | 4.218 | -7.811 | 1.00 | 23.54 | 6 |
| | ATOM | 1357 | O | VAL | A | 173 | 38.637 | 5.125 | -7.058 | 1.00 | 23.05 | 8 |
| | ATOM | 1358 | CB | VAL | A | 173 | 37.637 | 2.318 | -6.861 | 1.00 | 22.84 | 6 |
| | ATOM | 1359 | CG1 | VAL | A | 173 | 36.675 | 2.449 | -8.040 | 1.00 | 24.23 | 6 |
| | ATOM | 1360 | CG2 | VAL | A | 173 | 37.756 | 0.893 | -6.307 | 1.00 | 23.19 | 6 |
| 50 | ATOM | 1361 | N | GLY | A | 174 | 39.480 | 4.451 | -9.055 | 1.00 | 22.79 | 7 |
| | ATOM | 1362 | CA | GLY | A | 174 | 39.509 | 5.765 | -9.652 | 1.00 | 22.28 | 6 |
| | ATOM | 1363 | C | GLY | A | 174 | 38.217 | 5.872 | -10.462 | 1.00 | 25.76 | 6 |
| | ATOM | 1364 | O | GLY | A | 174 | 37.972 | 4.984 | -11.306 | 1.00 | 25.34 | 8 |
| | ATOM | 1365 | N | VAL | A | 175 | 37.340 | 6.803 | -10.087 | 1.00 | 22.69 | 7 |
| 55 | ATOM | 1366 | CA | VAL | A | 175 | 35.996 | 6.810 | -10.712 | 1.00 | 21.96 | 6 |
| | ATOM | 1367 | C | VAL | A | 175 | 36.025 | 7.779 | -11.858 | 1.00 | 22.74 | 6 |
| | ATOM | 1368 | O | VAL | A | 175 | 36.298 | 8.938 | -11.632 | 1.00 | 19.20 | 8 |
| | ATOM | 1369 | CB | VAL | A | 175 | 34.977 | 7.161 | -9.632 | 1.00 | 21.95 | 6 |
| | ATOM | 1370 | CG1 | VAL | A | 175 | 33.557 | 7.328 | -10.233 | 1.00 | 23.84 | 6 |
| 60 | ATOM | 1371 | CG2 | VAL | A | 175 | 34.914 | 6.111 | -8.501 | 1.00 | 20.67 | 6 |
| | ATOM | 1372 | N | PRO | A | 176 | 35.590 | 7.430 | -13.068 | 1.00 | 23.97 | 7 |
| | ATOM | 1373 | CA | PRO | A | 176 | 35.714 | 8.344 | -14.172 | 1.00 | 26.00 | 6 |
| | ATOM | 1374 | C | PRO | A | 176 | 34.750 | 9.485 | -14.090 | 1.00 | 23.25 | 6 |
| | ATOM | 1375 | O | PRO | A | 176 | 33.689 | 9.357 | -13.462 | 1.00 | 23.13 | 8 |
| 65 | ATOM | 1376 | CB | PRO | A | 176 | 35.429 | 7.464 | -15.401 | 1.00 | 26.90 | 6 |
| | ATOM | 1377 | CG | PRO | A | 176 | 35.554 | 6.062 | -14.946 | 1.00 | 30.42 | 6 |
| | ATOM | 1378 | CD | PRO | A | 176 | 35.214 | 6.053 | -13.467 | 1.00 | 26.21 | 6 |
| | ATOM | 1379 | N | ILE | A | 177 | 35.026 | 10.601 | -14.706 | 1.00 | 25.15 | 7 |
| | ATOM | 1380 | CA | ILE | A | 177 | 34.220 | 11.792 | -14.882 | 1.00 | 25.60 | 6 |
| 70 | ATOM | 1381 | C | ILE | A | 177 | 32.858 | 11.452 | -15.470 | 1.00 | 26.15 | 6 |
| | ATOM | 1382 | O | ILE | A | 177 | 32.823 | 10.610 | -16.392 | 1.00 | 25.13 | 8 |
| | ATOM | 1383 | CB | ILE | A | 177 | 35.002 | 12.755 | -15.816 | 1.00 | 27.16 | 6 |
| | ATOM | 1384 | CG1 | ILE | A | 177 | 36.095 | 13.432 | -14.910 | 1.00 | 32.12 | 6 |
| | ATOM | 1385 | CG2 | ILE | A | 177 | 34.203 | 13.794 | -16.565 | 1.00 | 27.48 | 6 |
| | ATOM | 1386 | CD1 | ILE | A | 177 | 37.253 | 13.907 | -15.774 | 1.00 | 33.86 | 6 |

-55-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|----|
| | ATOM | 1387 | N | MET | A | 178 | 31.789 | 11.892 | -14.839 | 1.00 | 23.56 | 7 |
| | ATOM | 1388 | CA | MET | A | 178 | 30.439 | 11.695 | -15.338 | 1.00 | 22.41 | 6 |
| | ATOM | 1389 | C | MET | A | 178 | 30.253 | 12.624 | -16.564 | 1.00 | 19.13 | 6 |
| 5 | ATOM | 1390 | O | MET | A | 178 | 30.623 | 13.780 | -16.493 | 1.00 | 19.54 | 8 |
| | ATOM | 1391 | CB | MET | A | 178 | 29.352 | 12.079 | -14.359 | 1.00 | 28.06 | 6 |
| | ATOM | 1392 | CG | MET | A | 178 | 29.443 | 11.331 | -13.018 | 1.00 | 34.50 | 6 |
| | ATOM | 1393 | SD | MET | A | 178 | 28.135 | 11.774 | -11.868 | 1.00 | 41.82 | 16 |
| | ATOM | 1394 | CE | MET | A | 178 | 28.027 | 13.573 | -11.994 | 1.00 | 44.07 | 6 |
| 10 | ATOM | 1395 | N | ARG | A | 179 | 29.559 | 12.130 | -17.573 | 1.00 | 19.57 | 7 |
| | ATOM | 1396 | CA | ARG | A | 179 | 29.384 | 12.934 | -18.776 | 1.00 | 18.81 | 6 |
| | ATOM | 1397 | C | ARG | A | 179 | 27.950 | 12.914 | -19.257 | 1.00 | 19.43 | 6 |
| | ATOM | 1398 | O | ARG | A | 179 | 27.182 | 12.014 | -18.938 | 1.00 | 19.78 | 8 |
| | ATOM | 1399 | CB | ARG | A | 179 | 30.252 | 12.380 | -19.936 | 1.00 | 20.44 | 6 |
| 15 | ATOM | 1400 | CG | ARG | A | 179 | 31.757 | 12.403 | -19.680 | 1.00 | 21.94 | 6 |
| | ATOM | 1401 | CD | ARG | A | 179 | 32.547 | 11.665 | -20.791 | 1.00 | 22.96 | 6 |
| | ATOM | 1402 | NE | ARG | A | 179 | 33.928 | 11.849 | -20.377 | 1.00 | 24.17 | 7 |
| | ATOM | 1403 | CZ | ARG | A | 179 | 34.636 | 12.995 | -20.379 | 1.00 | 23.08 | 6 |
| | ATOM | 1404 | NH1 | ARG | A | 179 | 34.146 | 14.147 | -20.883 | 1.00 | 22.58 | 7 |
| 20 | ATOM | 1405 | NH2 | ARG | A | 179 | 35.872 | 12.925 | -19.895 | 1.00 | 25.87 | 7 |
| | ATOM | 1406 | N | ALA | A | 180 | 27.526 | 13.954 | -19.931 | 1.00 | 19.29 | 7 |
| | ATOM | 1407 | CA | ALA | A | 180 | 26.247 | 14.023 | -20.609 | 1.00 | 20.57 | 6 |
| | ATOM | 1408 | C | ALA | A | 180 | 26.269 | 13.017 | -21.785 | 1.00 | 20.46 | 6 |
| | ATOM | 1409 | O | ALA | A | 180 | 27.305 | 12.438 | -22.089 | 1.00 | 20.53 | 8 |
| 25 | ATOM | 1410 | CB | ALA | A | 180 | 26.009 | 15.430 | -21.100 | 1.00 | 20.95 | 6 |
| | ATOM | 1411 | N | LYS | A | 181 | 25.065 | 12.823 | -22.355 | 1.00 | 23.00 | 7 |
| | ATOM | 1412 | CA | LYS | A | 181 | 24.978 | 11.807 | -23.436 | 1.00 | 25.24 | 6 |
| | ATOM | 1413 | C | LYS | A | 181 | 25.745 | 12.150 | -24.672 | 1.00 | 23.73 | 6 |
| | ATOM | 1414 | O | LYS | A | 181 | 26.108 | 11.238 | -25.439 | 1.00 | 25.08 | 8 |
| | ATOM | 1415 | CB | LYS | A | 181 | 23.496 | 11.637 | -23.802 | 1.00 | 25.36 | 6 |
| 30 | ATOM | 1416 | CG | LYS | A | 181 | 22.670 | 10.939 | -22.755 | 1.00 | 29.60 | 6 |
| | ATOM | 1417 | CD | LYS | A | 181 | 23.217 | 9.642 | -22.291 | 1.00 | 31.75 | 6 |
| | ATOM | 1418 | N | ASP | A | 182 | 26.027 | 13.427 | -24.854 | 1.00 | 22.41 | 7 |
| | ATOM | 1419 | CA | ASP | A | 182 | 26.844 | 13.896 | -25.958 | 1.00 | 23.30 | 6 |
| 35 | ATOM | 1420 | C | ASP | A | 182 | 28.319 | 13.944 | -25.618 | 1.00 | 24.01 | 6 |
| | ATOM | 1421 | O | ASP | A | 182 | 29.102 | 14.328 | -26.481 | 1.00 | 23.06 | 8 |
| | ATOM | 1422 | CB | ASP | A | 182 | 26.269 | 15.241 | -26.435 | 1.00 | 23.96 | 6 |
| | ATOM | 1423 | CG | ASP | A | 182 | 26.307 | 16.365 | -25.427 | 1.00 | 25.62 | 6 |
| | ATOM | 1424 | OD1 | ASP | A | 182 | 26.954 | 16.241 | -24.359 | 1.00 | 24.83 | 8 |
| 40 | ATOM | 1425 | OD2 | ASP | A | 182 | 25.690 | 17.397 | -25.755 | 1.00 | 27.42 | 8 |
| | ATOM | 1426 | N | GLY | A | 183 | 28.808 | 13.557 | -24.413 | 1.00 | 19.95 | 7 |
| | ATOM | 1427 | CA | GLY | A | 183 | 30.201 | 13.464 | -24.071 | 1.00 | 23.13 | 6 |
| | ATOM | 1428 | C | GLY | A | 183 | 30.666 | 14.607 | -23.127 | 1.00 | 19.95 | 6 |
| | ATOM | 1429 | O | GLY | A | 183 | 31.799 | 14.532 | -22.661 | 1.00 | 21.39 | 8 |
| 45 | ATOM | 1430 | N | LEU | A | 184 | 29.882 | 15.681 | -23.119 | 1.00 | 19.14 | 7 |
| | ATOM | 1431 | CA | LEU | A | 184 | 30.339 | 16.847 | -22.301 | 1.00 | 18.16 | 6 |
| | ATOM | 1432 | C | LEU | A | 184 | 30.494 | 16.470 | -20.832 | 1.00 | 18.40 | 6 |
| | ATOM | 1433 | O | LEU | A | 184 | 29.587 | 15.913 | -20.225 | 1.00 | 19.97 | 8 |
| | ATOM | 1434 | CB | LEU | A | 184 | 29.377 | 18.028 | -22.486 | 1.00 | 18.63 | 6 |
| 50 | ATOM | 1435 | CG | LEU | A | 184 | 29.738 | 19.280 | -21.652 | 1.00 | 17.34 | 6 |
| | ATOM | 1436 | CD1 | LEU | A | 184 | 31.065 | 19.909 | -22.111 | 1.00 | 19.12 | 6 |
| | ATOM | 1437 | CD2 | LEU | A | 184 | 28.615 | 20.311 | -21.740 | 1.00 | 19.88 | 6 |
| | ATOM | 1438 | N | ALA | A | 185 | 31.607 | 16.870 | -20.184 | 1.00 | 16.12 | 7 |
| | ATOM | 1439 | CA | ALA | A | 185 | 31.782 | 16.555 | -18.761 | 1.00 | 18.63 | 6 |
| 55 | ATOM | 1440 | C | ALA | A | 185 | 30.744 | 17.337 | -17.942 | 1.00 | 17.79 | 6 |
| | ATOM | 1441 | O | ALA | A | 185 | 30.537 | 18.511 | -18.196 | 1.00 | 18.57 | 8 |
| | ATOM | 1442 | CB | ALA | A | 185 | 33.237 | 16.872 | -18.396 | 1.00 | 20.34 | 6 |
| | ATOM | 1443 | N | LEU | A | 186 | 30.024 | 16.634 | -17.065 | 1.00 | 16.87 | 7 |
| | ATOM | 1444 | CA | LEU | A | 186 | 29.020 | 17.352 | -16.271 | 1.00 | 16.99 | 6 |
| 60 | ATOM | 1445 | C | LEU | A | 186 | 29.790 | 18.284 | -15.327 | 1.00 | 17.67 | 6 |
| | ATOM | 1446 | O | LEU | A | 186 | 30.768 | 17.866 | -14.658 | 1.00 | 20.34 | 8 |
| | ATOM | 1447 | CB | LEU | A | 186 | 28.117 | 16.384 | -15.513 | 1.00 | 16.87 | 6 |
| | ATOM | 1448 | CG | LEU | A | 186 | 27.300 | 15.408 | -16.358 | 1.00 | 18.67 | 6 |
| | ATOM | 1449 | CD1 | LEU | A | 186 | 26.353 | 14.626 | -15.456 | 1.00 | 20.67 | 6 |
| 65 | ATOM | 1450 | CD2 | LEU | A | 186 | 26.520 | 16.166 | -17.415 | 1.00 | 17.31 | 6 |
| | ATOM | 1451 | N | SER | A | 187 | 29.252 | 19.481 | -15.220 | 1.00 | 18.83 | 7 |
| | ATOM | 1452 | CA | SER | A | 187 | 29.915 | 20.486 | -14.382 | 1.00 | 17.18 | 6 |
| | ATOM | 1453 | C | SER | A | 187 | 29.000 | 21.631 | -14.105 | 1.00 | 17.64 | 6 |
| | ATOM | 1454 | O | SER | A | 187 | 28.216 | 22.057 | -14.964 | 1.00 | 18.63 | 8 |
| 70 | ATOM | 1455 | CB | SER | A | 187 | 31.153 | 21.021 | -15.151 | 1.00 | 20.23 | 6 |
| | ATOM | 1456 | OG | SER | A | 187 | 31.730 | 22.134 | -14.430 | 1.00 | 20.91 | 8 |
| | ATOM | 1457 | N | SER | A | 188 | 29.176 | 22.275 | -12.905 | 1.00 | 17.55 | 7 |
| | ATOM | 1458 | CA | SER | A | 188 | 28.463 | 23.548 | -12.722 | 1.00 | 17.70 | 6 |
| | ATOM | 1459 | C | SER | A | 188 | 28.806 | 24.605 | -13.755 | 1.00 | 17.74 | 6 |
| | ATOM | 1460 | O | SER | A | 188 | 28.014 | 25.522 | -14.095 | 1.00 | 18.92 | 8 |

-56-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1461 | CB | SER | A | 188 | 28.799 | 24.124 | -11.327 | 1.00 | 19.73 | 6 |
| | ATOM | 1462 | OG | SER | A | 188 | 30.220 | 24.296 | -11.200 | 1.00 | 20.84 | 8 |
| | ATOM | 1463 | N | ARG | A | 189 | 29.969 | 24.554 | -14.393 | 1.00 | 18.16 | 7 |
| 5 | ATOM | 1464 | CA | ARG | A | 189 | 30.424 | 25.497 | -15.393 | 1.00 | 19.85 | 6 |
| | ATOM | 1465 | C | ARG | A | 189 | 29.538 | 25.498 | -16.634 | 1.00 | 20.33 | 6 |
| | ATOM | 1466 | O | ARG | A | 189 | 29.484 | 26.473 | -17.348 | 1.00 | 21.91 | 8 |
| | ATOM | 1467 | CB | ARG | A | 189 | 31.879 | 25.201 | -15.823 | 1.00 | 20.55 | 6 |
| | ATOM | 1468 | CG | ARG | A | 189 | 32.801 | 25.314 | -14.605 | 1.00 | 22.89 | 6 |
| 10 | ATOM | 1469 | CD | ARG | A | 189 | 34.254 | 25.061 | -15.042 | 1.00 | 23.21 | 6 |
| | ATOM | 1470 | NE | ARG | A | 189 | 35.037 | 25.170 | -13.785 | 1.00 | 25.97 | 7 |
| | ATOM | 1471 | CZ | ARG | A | 189 | 36.121 | 25.924 | -13.683 | 1.00 | 28.29 | 6 |
| | ATOM | 1472 | NH1 | ARG | A | 189 | 36.608 | 26.564 | -14.711 | 1.00 | 26.60 | 7 |
| | ATOM | 1473 | NH2 | ARG | A | 189 | 36.744 | 25.966 | -12.487 | 1.00 | 28.41 | 7 |
| 15 | ATOM | 1474 | N | ASN | A | 190 | 28.914 | 24.324 | -16.956 | 1.00 | 19.42 | 7 |
| | ATOM | 1475 | CA | ASN | A | 190 | 28.105 | 24.261 | -18.156 | 1.00 | 19.64 | 6 |
| | ATOM | 1476 | C | ASN | A | 190 | 26.963 | 25.235 | -18.114 | 1.00 | 22.61 | 6 |
| | ATOM | 1477 | O | ASN | A | 190 | 26.271 | 25.606 | -19.109 | 1.00 | 23.27 | 8 |
| | ATOM | 1478 | CB | ASN | A | 190 | 27.544 | 22.841 | -18.332 | 1.00 | 19.54 | 6 |
| 20 | ATOM | 1479 | CG | ASN | A | 190 | 28.675 | 21.842 | -18.530 | 1.00 | 21.41 | 6 |
| | ATOM | 1480 | OD1 | ASN | A | 190 | 28.471 | 20.621 | -18.265 | 1.00 | 21.40 | 8 |
| | ATOM | 1481 | ND2 | ASN | A | 190 | 29.819 | 22.309 | -18.997 | 1.00 | 19.16 | 7 |
| | ATOM | 1497 | N | GLY | A | 191 | 26.554 | 25.616 | -16.760 | 1.00 | 27.44 | 7 |
| | ATOM | 1498 | CA | GLY | A | 191 | 25.459 | 26.574 | -16.600 | 1.00 | 28.04 | 6 |
| 25 | ATOM | 1499 | C | GLY | A | 191 | 25.750 | 27.966 | -17.117 | 1.00 | 29.70 | 6 |
| | ATOM | 1500 | O | GLY | A | 191 | 24.790 | 28.715 | -17.294 | 1.00 | 31.47 | 8 |
| | ATOM | 1482 | N | TYR | A | 192 | 26.966 | 28.311 | -17.457 | 1.00 | 26.92 | 7 |
| | ATOM | 1483 | CA | TYR | A | 192 | 27.272 | 29.642 | -17.970 | 1.00 | 29.88 | 6 |
| | ATOM | 1484 | C | TYR | A | 192 | 27.308 | 29.633 | -19.479 | 1.00 | 29.91 | 6 |
| 30 | ATOM | 1485 | O | TYR | A | 192 | 27.538 | 30.724 | -20.046 | 1.00 | 34.28 | 8 |
| | ATOM | 1486 | CB | TYR | A | 192 | 28.611 | 30.173 | -17.427 | 1.00 | 30.32 | 6 |
| | ATOM | 1487 | CG | TYR | A | 192 | 28.459 | 30.366 | -15.928 | 1.00 | 32.17 | 6 |
| | ATOM | 1488 | CD1 | TYR | A | 192 | 28.608 | 29.256 | -15.102 | 1.00 | 32.38 | 6 |
| | ATOM | 1489 | CD2 | TYR | A | 192 | 28.097 | 31.585 | -15.362 | 1.00 | 34.00 | 6 |
| 35 | ATOM | 1490 | CE1 | TYR | A | 192 | 28.438 | 29.352 | -13.751 | 1.00 | 35.21 | 6 |
| | ATOM | 1491 | CE2 | TYR | A | 192 | 27.927 | 31.687 | -13.985 | 1.00 | 34.55 | 6 |
| | ATOM | 1492 | CZ | TYR | A | 192 | 28.106 | 30.589 | -13.195 | 1.00 | 36.66 | 6 |
| | ATOM | 1493 | OH | TYR | A | 192 | 27.942 | 30.636 | -11.819 | 1.00 | 38.33 | 8 |
| | ATOM | 1494 | N | LEU | A | 193 | 27.090 | 28.487 | -20.135 | 1.00 | 28.20 | 7 |
| 40 | ATOM | 1495 | CA | LEU | A | 193 | 27.054 | 28.479 | -21.575 | 1.00 | 26.63 | 6 |
| | ATOM | 1496 | C | LEU | A | 193 | 25.718 | 28.903 | -22.154 | 1.00 | 27.15 | 6 |
| | ATOM | 1497 | O | LEU | A | 193 | 24.697 | 28.434 | -21.647 | 1.00 | 28.28 | 8 |
| | ATOM | 1498 | CB | LEU | A | 193 | 27.315 | 27.057 | -22.112 | 1.00 | 26.20 | 6 |
| | ATOM | 1499 | CG | LEU | A | 193 | 28.613 | 26.402 | -21.654 | 1.00 | 25.58 | 6 |
| 45 | ATOM | 1500 | CD1 | LEU | A | 193 | 28.593 | 24.905 | -21.877 | 1.00 | 24.08 | 6 |
| | ATOM | 1501 | CD2 | LEU | A | 193 | 29.827 | 27.005 | -22.390 | 1.00 | 27.77 | 6 |
| | ATOM | 1502 | N | THR | A | 194 | 25.679 | 29.616 | -23.303 | 1.00 | 28.42 | 7 |
| | ATOM | 1503 | CA | THR | A | 194 | 24.376 | 29.825 | -23.934 | 1.00 | 27.62 | 6 |
| | ATOM | 1504 | C | THR | A | 194 | 23.892 | 28.531 | -24.561 | 1.00 | 25.74 | 6 |
| 50 | ATOM | 1505 | O | THR | A | 194 | 24.735 | 27.621 | -24.723 | 1.00 | 26.48 | 8 |
| | ATOM | 1506 | CB | THR | A | 194 | 24.463 | 30.922 | -25.011 | 1.00 | 29.34 | 6 |
| | ATOM | 1507 | OG1 | THR | A | 194 | 25.465 | 30.535 | -25.956 | 1.00 | 30.55 | 8 |
| | ATOM | 1508 | CG2 | THR | A | 194 | 24.862 | 32.238 | -24.353 | 1.00 | 32.65 | 6 |
| | ATOM | 1509 | N | ALA | A | 195 | 22.663 | 28.446 | -25.043 | 1.00 | 25.15 | 7 |
| 55 | ATOM | 1510 | CA | ALA | A | 195 | 22.211 | 27.253 | -25.755 | 1.00 | 25.73 | 6 |
| | ATOM | 1511 | C | ALA | A | 195 | 23.105 | 26.994 | -26.972 | 1.00 | 28.33 | 6 |
| | ATOM | 1512 | O | ALA | A | 195 | 23.460 | 25.834 | -27.241 | 1.00 | 28.09 | 8 |
| | ATOM | 1513 | CB | ALA | A | 195 | 20.768 | 27.315 | -26.209 | 1.00 | 25.63 | 6 |
| | ATOM | 1514 | N | GLU | A | 196 | 23.486 | 28.068 | -27.703 | 1.00 | 27.21 | 7 |
| 60 | ATOM | 1515 | CA | GLU | A | 196 | 24.366 | 27.886 | -28.843 | 1.00 | 28.84 | 6 |
| | ATOM | 1516 | C | GLU | A | 196 | 25.718 | 27.351 | -28.424 | 1.00 | 25.77 | 6 |
| | ATOM | 1517 | O | GLU | A | 196 | 26.282 | 26.445 | -29.054 | 1.00 | 30.10 | 8 |
| | ATOM | 1518 | CB | GLU | A | 196 | 24.534 | 29.239 | -29.570 | 1.00 | 31.35 | 6 |
| | ATOM | 1519 | N | GLN | A | 197 | 26.278 | 27.889 | -27.328 | 1.00 | 26.45 | 7 |
| 65 | ATOM | 1520 | CA | GLN | A | 197 | 27.567 | 27.412 | -26.855 | 1.00 | 25.85 | 6 |
| | ATOM | 1521 | C | GLN | A | 197 | 27.489 | 25.961 | -26.330 | 1.00 | 25.97 | 6 |
| | ATOM | 1522 | O | GLN | A | 197 | 28.406 | 25.210 | -26.618 | 1.00 | 25.79 | 8 |
| | ATOM | 1523 | CB | GLN | A | 197 | 28.157 | 28.273 | -25.717 | 1.00 | 27.14 | 6 |
| | ATOM | 1524 | CG | GLN | A | 197 | 28.452 | 29.662 | -26.408 | 1.00 | 29.94 | 6 |
| 70 | ATOM | 1525 | CD | GLN | A | 197 | 28.544 | 30.739 | -25.358 | 1.00 | 31.03 | 6 |
| | ATOM | 1526 | OE1 | GLN | A | 197 | 28.249 | 30.597 | -24.174 | 1.00 | 31.48 | 8 |
| | ATOM | 1527 | NE2 | GLN | A | 197 | 28.949 | 31.963 | -25.739 | 1.00 | 30.58 | 7 |
| | ATOM | 1528 | N | ARG | A | 198 | 26.335 | 25.639 | -25.736 | 1.00 | 23.62 | 7 |
| | ATOM | 1529 | CA | ARG | A | 198 | 26.151 | 24.282 | -25.209 | 1.00 | 23.58 | 6 |
| | ATOM | 1530 | C | ARG | A | 198 | 26.204 | 23.282 | -26.345 | 1.00 | 24.98 | 6 |

-57-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1531 | O | ARG | A | 198 | 26.761 | 22.214 | -26.214 | 1.00 | 25.17 | 8 |
| | ATOM | 1532 | CB | ARG | A | 198 | 24.831 | 24.133 | -24.454 | 1.00 | 22.16 | 6 |
| | ATOM | 1533 | CG | ARG | A | 198 | 24.576 | 22.689 | -23.946 | 1.00 | 21.81 | 6 |
| | ATOM | 1534 | CD | ARG | A | 198 | 25.656 | 22.194 | -23.010 | 1.00 | 22.56 | 6 |
| 5 | ATOM | 1535 | NE | ARG | A | 198 | 25.386 | 20.830 | -22.532 | 1.00 | 21.88 | 7 |
| | ATOM | 1536 | CZ | ARG | A | 198 | 25.614 | 19.724 | -23.247 | 1.00 | 24.32 | 6 |
| | ATOM | 1537 | NH1 | ARG | A | 198 | 25.384 | 18.481 | -22.824 | 1.00 | 23.45 | 7 |
| | ATOM | 1538 | NH2 | ARG | A | 198 | 26.118 | 19.830 | -24.477 | 1.00 | 25.14 | 7 |
| 10 | ATOM | 1539 | N | LYS | A | 199 | 25.707 | 23.649 | -27.549 | 1.00 | 23.80 | 7 |
| | ATOM | 1540 | CA | LYS | A | 199 | 25.820 | 22.710 | -28.684 | 1.00 | 22.66 | 6 |
| | ATOM | 1541 | C | LYS | A | 199 | 27.221 | 22.558 | -29.202 | 1.00 | 22.59 | 6 |
| | ATOM | 1542 | O | LYS | A | 199 | 27.608 | 21.508 | -29.753 | 1.00 | 24.00 | 8 |
| | ATOM | 1543 | CB | LYS | A | 199 | 24.855 | 23.272 | -29.743 | 1.00 | 25.23 | 6 |
| | ATOM | 1544 | CG | LYS | A | 199 | 24.661 | 22.284 | -30.903 | 1.00 | 27.40 | 6 |
| 15 | ATOM | 1545 | CD | LYS | A | 199 | 23.602 | 22.991 | -31.802 | 1.00 | 32.35 | 6 |
| | ATOM | 1546 | CE | LYS | A | 199 | 23.336 | 22.059 | -32.983 | 1.00 | 36.02 | 6 |
| | ATOM | 1547 | NZ | LYS | A | 199 | 22.311 | 22.674 | -33.894 | 1.00 | 38.59 | 7 |
| | ATOM | 1548 | N | ILE | A | 200 | 28.111 | 23.556 | -29.074 | 1.00 | 22.04 | 7 |
| 20 | ATOM | 1549 | CA | ILE | A | 200 | 29.513 | 23.458 | -29.440 | 1.00 | 25.05 | 6 |
| | ATOM | 1550 | C | ILE | A | 200 | 30.415 | 22.725 | -28.438 | 1.00 | 23.70 | 6 |
| | ATOM | 1551 | O | ILE | A | 200 | 31.347 | 21.980 | -28.775 | 1.00 | 22.15 | 8 |
| | ATOM | 1552 | CB | ILE | A | 200 | 30.128 | 24.863 | -29.575 | 1.00 | 25.43 | 6 |
| | ATOM | 1553 | CG1 | ILE | A | 200 | 29.457 | 25.528 | -30.809 | 1.00 | 26.99 | 6 |
| 25 | ATOM | 1554 | CG2 | ILE | A | 200 | 31.644 | 24.911 | -29.704 | 1.00 | 26.61 | 6 |
| | ATOM | 1555 | CD1 | ILE | A | 200 | 29.746 | 27.029 | -30.827 | 1.00 | 28.65 | 6 |
| | ATOM | 1556 | N | ALA | A | 201 | 29.987 | 22.836 | -27.170 | 1.00 | 22.88 | 7 |
| | ATOM | 1557 | CA | ALA | A | 201 | 30.773 | 22.278 | -26.053 | 1.00 | 24.80 | 6 |
| | ATOM | 1558 | C | ALA | A | 201 | 31.217 | 20.829 | -26.110 | 1.00 | 23.52 | 6 |
| 30 | ATOM | 1559 | O | ALA | A | 201 | 32.363 | 20.607 | -25.709 | 1.00 | 21.96 | 8 |
| | ATOM | 1560 | CB | ALA | A | 201 | 29.913 | 22.499 | -24.781 | 1.00 | 24.70 | 6 |
| | ATOM | 1561 | N | PRO | A | 202 | 30.498 | 19.846 | -26.659 | 1.00 | 24.18 | 7 |
| | ATOM | 1562 | CA | PRO | A | 202 | 30.946 | 18.473 | -26.796 | 1.00 | 24.19 | 6 |
| | ATOM | 1563 | C | PRO | A | 202 | 32.191 | 18.288 | -27.649 | 1.00 | 26.04 | 6 |
| 35 | ATOM | 1564 | O | PRO | A | 202 | 32.900 | 17.282 | -27.556 | 1.00 | 25.77 | 8 |
| | ATOM | 1565 | CB | PRO | A | 202 | 29.759 | 17.693 | -27.382 | 1.00 | 24.31 | 6 |
| | ATOM | 1566 | CG | PRO | A | 202 | 28.579 | 18.572 | -27.068 | 1.00 | 23.02 | 6 |
| | ATOM | 1567 | CD | PRO | A | 202 | 29.073 | 19.991 | -27.051 | 1.00 | 22.33 | 6 |
| | ATOM | 1568 | N | GLY | A | 203 | 32.559 | 19.351 | -28.406 | 1.00 | 25.61 | 7 |
| 40 | ATOM | 1569 | CA | GLY | A | 203 | 33.779 | 19.327 | -29.179 | 1.00 | 26.22 | 6 |
| | ATOM | 1570 | C | GLY | A | 203 | 35.012 | 19.196 | -28.324 | 1.00 | 24.81 | 6 |
| | ATOM | 1571 | O | GLY | A | 203 | 36.061 | 18.750 | -28.817 | 1.00 | 24.88 | 8 |
| | ATOM | 1572 | N | LEU | A | 204 | 34.999 | 19.724 | -27.082 | 1.00 | 23.90 | 7 |
| | ATOM | 1573 | CA | LEU | A | 204 | 36.199 | 19.561 | -26.254 | 1.00 | 23.72 | 6 |
| 45 | ATOM | 1574 | C | LEU | A | 204 | 36.550 | 18.119 | -26.035 | 1.00 | 23.32 | 6 |
| | ATOM | 1575 | O | LEU | A | 204 | 37.689 | 17.689 | -26.239 | 1.00 | 24.33 | 8 |
| | ATOM | 1576 | CB | LEU | A | 204 | 35.957 | 20.361 | -24.936 | 1.00 | 24.53 | 6 |
| | ATOM | 1577 | CG | LEU | A | 204 | 37.111 | 20.290 | -23.972 | 1.00 | 25.84 | 6 |
| | ATOM | 1578 | CD1 | LEU | A | 204 | 38.425 | 20.791 | -24.586 | 1.00 | 26.75 | 6 |
| 50 | ATOM | 1579 | CD2 | LEU | A | 204 | 36.806 | 21.156 | -22.742 | 1.00 | 26.68 | 6 |
| | ATOM | 1580 | N | TYR | A | 205 | 35.580 | 17.243 | -25.663 | 1.00 | 21.57 | 7 |
| | ATOM | 1581 | CA | TYR | A | 205 | 35.804 | 15.836 | -25.435 | 1.00 | 22.36 | 6 |
| | ATOM | 1582 | C | TYR | A | 205 | 36.200 | 15.116 | -26.748 | 1.00 | 21.69 | 6 |
| | ATOM | 1583 | O | TYR | A | 205 | 37.041 | 14.212 | -26.762 | 1.00 | 23.95 | 8 |
| 55 | ATOM | 1584 | CB | TYR | A | 205 | 34.533 | 15.211 | -24.809 | 1.00 | 21.96 | 6 |
| | ATOM | 1585 | CG | TYR | A | 205 | 34.766 | 13.758 | -24.505 | 1.00 | 25.55 | 6 |
| | ATOM | 1586 | CD1 | TYR | A | 205 | 35.727 | 13.322 | -23.619 | 1.00 | 27.86 | 6 |
| | ATOM | 1587 | CD2 | TYR | A | 205 | 34.059 | 12.802 | -25.253 | 1.00 | 29.16 | 6 |
| | ATOM | 1588 | CE1 | TYR | A | 205 | 35.901 | 11.979 | -23.364 | 1.00 | 30.07 | 6 |
| 60 | ATOM | 1589 | CE2 | TYR | A | 205 | 34.261 | 11.448 | -25.003 | 1.00 | 30.89 | 6 |
| | ATOM | 1590 | CZ | TYR | A | 205 | 35.158 | 11.053 | -24.064 | 1.00 | 32.67 | 6 |
| | ATOM | 1591 | OH | TYR | A | 205 | 35.373 | 9.702 | -23.839 | 1.00 | 36.20 | 8 |
| | ATOM | 1592 | N | LYS | A | 206 | 35.652 | 15.679 | -27.833 | 1.00 | 23.35 | 7 |
| | ATOM | 1593 | CA | LYS | A | 206 | 36.040 | 15.114 | -29.149 | 1.00 | 24.75 | 6 |
| 65 | ATOM | 1594 | C | LYS | A | 206 | 37.530 | 15.306 | -29.401 | 1.00 | 24.74 | 6 |
| | ATOM | 1595 | O | LYS | A | 206 | 38.252 | 14.359 | -29.757 | 1.00 | 26.16 | 8 |
| | ATOM | 1596 | CB | LYS | A | 206 | 35.223 | 15.740 | -30.293 | 1.00 | 25.21 | 6 |
| | ATOM | 1597 | CG | LYS | A | 206 | 33.784 | 15.236 | -30.295 | 1.00 | 30.61 | 6 |
| | ATOM | 1598 | CD | LYS | A | 206 | 33.118 | 15.648 | -31.621 | 1.00 | 34.58 | 6 |
| | ATOM | 1599 | CE | LYS | A | 206 | 31.600 | 15.547 | -31.489 | 1.00 | 37.70 | 6 |
| 70 | ATOM | 1600 | NZ | LYS | A | 206 | 30.951 | 15.934 | -32.794 | 1.00 | 40.74 | 7 |
| | ATOM | 1601 | N | VAL | A | 207 | 37.995 | 16.518 | -29.128 | 1.00 | 25.56 | 7 |
| | ATOM | 1602 | CA | VAL | A | 207 | 39.432 | 16.818 | -29.324 | 1.00 | 26.41 | 6 |
| | ATOM | 1603 | C | VAL | A | 207 | 40.240 | 16.016 | -28.333 | 1.00 | 26.75 | 6 |
| | ATOM | 1604 | O | VAL | A | 207 | 41.246 | 15.351 | -28.662 | 1.00 | 26.06 | 8 |

-58-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1605 | CB | VAL | A | 207 | 39.714 | 18.318 | -29.266 | 1.00 | 26.88 | 6 |
| | ATOM | 1606 | CG1 | VAL | A | 207 | 41.212 | 18.590 | -29.172 | 1.00 | 27.69 | 6 |
| | ATOM | 1607 | CG2 | VAL | A | 207 | 39.062 | 18.967 | -30.489 | 1.00 | 27.15 | 6 |
| 5 | ATOM | 1608 | N | LEU | A | 208 | 39.793 | 15.917 | -27.065 | 1.00 | 26.81 | 7 |
| | ATOM | 1609 | CA | LEU | A | 208 | 40.472 | 15.110 | -26.079 | 1.00 | 26.80 | 6 |
| | ATOM | 1610 | C | LEU | A | 208 | 40.555 | 13.645 | -26.462 | 1.00 | 27.53 | 6 |
| | ATOM | 1611 | O | LEU | A | 208 | 41.616 | 13.017 | -26.276 | 1.00 | 27.79 | 8 |
| | ATOM | 1612 | CB | LEU | A | 208 | 39.736 | 15.325 | -24.732 | 1.00 | 28.31 | 6 |
| 10 | ATOM | 1613 | CG | LEU | A | 208 | 40.248 | 14.531 | -23.535 | 1.00 | 31.14 | 6 |
| | ATOM | 1614 | CD1 | LEU | A | 208 | 41.649 | 14.906 | -23.142 | 1.00 | 31.37 | 6 |
| | ATOM | 1615 | CD2 | LEU | A | 208 | 39.288 | 14.741 | -22.347 | 1.00 | 33.29 | 6 |
| | ATOM | 1616 | N | SER | A | 209 | 39.539 | 13.042 | -27.028 | 1.00 | 26.96 | 7 |
| | ATOM | 1617 | CA | SER | A | 209 | 39.536 | 11.655 | -27.442 | 1.00 | 28.65 | 6 |
| 15 | ATOM | 1618 | C | SER | A | 209 | 40.427 | 11.463 | -28.696 | 1.00 | 30.30 | 6 |
| | ATOM | 1619 | O | SER | A | 209 | 41.021 | 10.401 | -28.829 | 1.00 | 29.86 | 8 |
| | ATOM | 1620 | CB | SER | A | 209 | 38.141 | 11.126 | -27.751 | 1.00 | 32.08 | 6 |
| | ATOM | 1621 | OG | SER | A | 209 | 37.320 | 11.455 | -26.630 | 1.00 | 36.96 | 8 |
| | ATOM | 1622 | N | SER | A | 210 | 40.502 | 12.521 | -29.507 | 1.00 | 31.09 | 7 |
| 20 | ATOM | 1623 | CA | SER | A | 210 | 41.372 | 12.426 | -30.703 | 1.00 | 33.89 | 6 |
| | ATOM | 1624 | C | SER | A | 210 | 42.826 | 12.447 | -30.297 | 1.00 | 33.77 | 6 |
| | ATOM | 1625 | O | SER | A | 210 | 43.687 | 11.734 | -30.842 | 1.00 | 34.87 | 8 |
| | ATOM | 1626 | CB | SER | A | 210 | 41.024 | 13.563 | -31.655 | 1.00 | 36.51 | 6 |
| | ATOM | 1627 | OG | SER | A | 210 | 42.171 | 13.743 | -32.490 | 1.00 | 42.40 | 8 |
| 25 | ATOM | 1628 | N | ILE | A | 211 | 43.172 | 13.190 | -29.230 | 1.00 | 31.25 | 7 |
| | ATOM | 1629 | CA | ILE | A | 211 | 44.530 | 13.129 | -28.705 | 1.00 | 30.79 | 6 |
| | ATOM | 1630 | C | ILE | A | 211 | 44.815 | 11.731 | -28.188 | 1.00 | 31.65 | 6 |
| | ATOM | 1631 | O | ILE | A | 211 | 45.878 | 11.124 | -28.405 | 1.00 | 31.20 | 8 |
| | ATOM | 1632 | CB | ILE | A | 211 | 44.710 | 14.154 | -27.580 | 1.00 | 30.45 | 6 |
| 30 | ATOM | 1633 | CG1 | ILE | A | 211 | 44.646 | 15.580 | -28.137 | 1.00 | 29.16 | 6 |
| | ATOM | 1634 | CG2 | ILE | A | 211 | 46.009 | 13.912 | -26.797 | 1.00 | 28.20 | 6 |
| | ATOM | 1635 | CD1 | ILE | A | 211 | 44.501 | 16.613 | -27.014 | 1.00 | 28.78 | 6 |
| | ATOM | 1636 | N | ALA | A | 212 | 43.882 | 11.162 | -27.426 | 1.00 | 31.19 | 7 |
| | ATOM | 1637 | CA | ALA | A | 212 | 44.069 | 9.828 | -26.852 | 1.00 | 31.19 | 6 |
| 35 | ATOM | 1638 | C | ALA | A | 212 | 44.251 | 8.789 | -27.955 | 1.00 | 33.70 | 6 |
| | ATOM | 1639 | O | ALA | A | 212 | 45.100 | 7.892 | -27.832 | 1.00 | 34.72 | 8 |
| | ATOM | 1640 | CB | ALA | A | 212 | 42.879 | 9.427 | -25.995 | 1.00 | 31.27 | 6 |
| | ATOM | 1641 | N | ASP | A | 213 | 43.478 | 8.916 | -29.045 | 1.00 | 32.83 | 7 |
| | ATOM | 1642 | CA | ASP | A | 213 | 43.576 | 7.982 | -30.167 | 1.00 | 34.55 | 6 |
| 40 | ATOM | 1643 | C | ASP | A | 213 | 45.008 | 7.998 | -30.723 | 1.00 | 34.80 | 6 |
| | ATOM | 1644 | O | ASP | A | 213 | 45.616 | 6.938 | -30.847 | 1.00 | 36.87 | 8 |
| | ATOM | 1645 | CB | ASP | A | 213 | 42.567 | 8.322 | -31.256 | 1.00 | 33.87 | 6 |
| | ATOM | 1646 | CG | ASP | A | 213 | 41.145 | 7.900 | -30.886 | 1.00 | 36.07 | 6 |
| | ATOM | 1647 | OD1 | ASP | A | 213 | 40.932 | 7.091 | -29.951 | 1.00 | 36.03 | 8 |
| 45 | ATOM | 1648 | OD2 | ASP | A | 213 | 40.224 | 8.400 | -31.585 | 1.00 | 36.99 | 8 |
| | ATOM | 1649 | N | LYS | A | 214 | 45.527 | 9.193 | -30.994 | 1.00 | 34.39 | 7 |
| | ATOM | 1650 | CA | LYS | A | 214 | 46.892 | 9.357 | -31.506 | 1.00 | 35.31 | 6 |
| | ATOM | 1651 | C | LYS | A | 214 | 47.904 | 8.782 | -30.536 | 1.00 | 37.91 | 6 |
| | ATOM | 1652 | O | LYS | A | 214 | 48.900 | 8.106 | -30.920 | 1.00 | 39.73 | 8 |
| 50 | ATOM | 1653 | CB | LYS | A | 214 | 47.196 | 10.833 | -31.789 | 1.00 | 33.06 | 6 |
| | ATOM | 1654 | CG | LYS | A | 214 | 46.295 | 11.525 | -32.774 | 1.00 | 33.68 | 6 |
| | ATOM | 1655 | CD | LYS | A | 214 | 46.733 | 12.968 | -33.079 | 1.00 | 32.27 | 6 |
| | ATOM | 1656 | CE | LYS | A | 214 | 45.891 | 13.544 | -34.215 | 1.00 | 33.88 | 6 |
| | ATOM | 1657 | NZ | LYS | A | 214 | 46.243 | 14.978 | -34.497 | 1.00 | 35.57 | 7 |
| 55 | ATOM | 1658 | N | LEU | A | 215 | 47.726 | 9.056 | -29.227 | 1.00 | 38.37 | 7 |
| | ATOM | 1659 | CA | LEU | A | 215 | 48.742 | 8.507 | -28.299 | 1.00 | 41.26 | 6 |
| | ATOM | 1660 | C | LEU | A | 215 | 48.676 | 6.988 | -28.267 | 1.00 | 42.76 | 6 |
| | ATOM | 1661 | O | LEU | A | 215 | 49.717 | 6.311 | -28.250 | 1.00 | 43.43 | 8 |
| | ATOM | 1662 | CB | LEU | A | 215 | 48.615 | 9.016 | -26.871 | 1.00 | 38.15 | 6 |
| 60 | ATOM | 1663 | CG | LEU | A | 215 | 48.941 | 10.483 | -26.658 | 1.00 | 39.14 | 6 |
| | ATOM | 1664 | CD1 | LEU | A | 215 | 48.406 | 10.973 | -25.306 | 1.00 | 39.20 | 6 |
| | ATOM | 1665 | CD2 | LEU | A | 215 | 50.441 | 10.749 | -26.718 | 1.00 | 39.00 | 6 |
| | ATOM | 1666 | N | GLN | A | 216 | 47.493 | 6.407 | -28.253 | 1.00 | 44.37 | 7 |
| | ATOM | 1667 | CA | GLN | A | 216 | 47.328 | 4.952 | -28.225 | 1.00 | 47.10 | 6 |
| 65 | ATOM | 1668 | C | GLN | A | 216 | 47.833 | 4.272 | -29.499 | 1.00 | 47.76 | 6 |
| | ATOM | 1669 | O | GLN | A | 216 | 48.153 | 3.081 | -29.469 | 1.00 | 48.80 | 8 |
| | ATOM | 1670 | CB | GLN | A | 216 | 45.859 | 4.643 | -27.991 | 1.00 | 48.55 | 6 |
| | ATOM | 1671 | CG | GLN | A | 216 | 45.452 | 3.303 | -27.435 | 1.00 | 50.81 | 6 |
| | ATOM | 1672 | CD | GLN | A | 216 | 44.259 | 3.444 | -26.493 | 1.00 | 53.17 | 6 |
| 70 | ATOM | 1673 | OE1 | GLN | A | 216 | 43.252 | 4.063 | -26.856 | 1.00 | 54.69 | 8 |
| | ATOM | 1674 | NE2 | GLN | A | 216 | 44.354 | 2.898 | -25.279 | 1.00 | 53.81 | 7 |
| | ATOM | 1675 | N | ALA | A | 217 | 47.944 | 4.977 | -30.617 | 1.00 | 47.64 | 7 |
| | ATOM | 1676 | CA | ALA | A | 217 | 48.431 | 4.433 | -31.869 | 1.00 | 48.49 | 6 |
| | ATOM | 1677 | C | ALA | A | 217 | 49.948 | 4.569 | -31.997 | 1.00 | 48.68 | 6 |
| | ATOM | 1678 | O | ALA | A | 217 | 50.517 | 4.182 | -33.024 | 1.00 | 51.00 | 8 |

-59-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1679 | CB | ALA | A | 217 | 47.789 | 5.138 | -33.060 | 1.00 | 47.71 | 6 |
| | ATOM | 1680 | N | GLY | A | 218 | 50.612 | 5.211 | -31.056 | 1.00 | 47.70 | 7 |
| | ATOM | 1681 | CA | GLY | A | 218 | 52.037 | 5.390 | -31.027 | 1.00 | 46.44 | 6 |
| 5 | ATOM | 1682 | C | GLY | A | 218 | 52.539 | 6.780 | -31.316 | 1.00 | 47.59 | 6 |
| | ATOM | 1683 | O | GLY | A | 218 | 53.771 | 6.979 | -31.285 | 1.00 | 47.50 | 8 |
| | ATOM | 1684 | N | GLU | A | 219 | 51.677 | 7.755 | -31.607 | 1.00 | 45.89 | 7 |
| | ATOM | 1685 | CA | GLU | A | 219 | 52.216 | 9.086 | -31.891 | 1.00 | 46.96 | 6 |
| | ATOM | 1686 | C | GLU | A | 219 | 52.912 | 9.624 | -30.651 | 1.00 | 48.26 | 6 |
| 10 | ATOM | 1687 | O | GLU | A | 219 | 52.403 | 9.484 | -29.530 | 1.00 | 48.86 | 8 |
| | ATOM | 1688 | CB | GLU | A | 219 | 51.146 | 10.071 | -32.380 | 1.00 | 47.88 | 6 |
| | ATOM | 1689 | CG | GLU | A | 219 | 50.460 | 9.695 | -33.672 | 1.00 | 48.05 | 6 |
| | ATOM | 1690 | CD | GLU | A | 219 | 49.744 | 10.817 | -34.384 | 1.00 | 50.68 | 6 |
| | ATOM | 1691 | OE1 | GLU | A | 219 | 50.134 | 12.015 | -34.408 | 1.00 | 51.01 | 8 |
| | ATOM | 1692 | OE2 | GLU | A | 219 | 48.702 | 10.497 | -35.025 | 1.00 | 52.09 | 8 |
| 15 | ATOM | 1693 | N | ARG | A | 220 | 54.135 | 10.154 | -30.831 | 1.00 | 47.68 | 7 |
| | ATOM | 1694 | CA | ARG | A | 220 | 54.868 | 10.698 | -29.694 | 1.00 | 47.37 | 6 |
| | ATOM | 1695 | C | ARG | A | 220 | 55.402 | 12.091 | -29.989 | 1.00 | 47.62 | 6 |
| | ATOM | 1696 | O | ARG | A | 220 | 56.106 | 12.622 | -29.125 | 1.00 | 49.49 | 8 |
| 20 | ATOM | 1697 | CB | ARG | A | 220 | 56.014 | 9.790 | -29.239 | 1.00 | 46.78 | 6 |
| | ATOM | 1698 | CG | ARG | A | 220 | 55.570 | 8.463 | -28.643 | 1.00 | 46.54 | 6 |
| | ATOM | 1699 | CD | ARG | A | 220 | 54.878 | 8.628 | -27.293 | 1.00 | 45.80 | 6 |
| | ATOM | 1700 | NE | ARG | A | 220 | 54.371 | 7.359 | -26.801 | 1.00 | 45.04 | 7 |
| | ATOM | 1701 | CZ | ARG | A | 220 | 53.281 | 6.683 | -27.074 | 1.00 | 44.93 | 6 |
| 25 | ATOM | 1702 | NH1 | ARG | A | 220 | 52.341 | 7.093 | -27.930 | 1.00 | 45.42 | 7 |
| | ATOM | 1703 | NH2 | ARG | A | 220 | 53.080 | 5.516 | -26.476 | 1.00 | 44.28 | 7 |
| | ATOM | 1704 | N | ASP | A | 221 | 54.976 | 12.756 | -31.052 | 1.00 | 48.60 | 7 |
| | ATOM | 1705 | CA | ASP | A | 221 | 55.381 | 14.161 | -31.242 | 1.00 | 48.15 | 6 |
| | ATOM | 1706 | C | ASP | A | 221 | 54.296 | 15.005 | -30.557 | 1.00 | 46.06 | 6 |
| 30 | ATOM | 1707 | O | ASP | A | 221 | 53.379 | 15.515 | -31.197 | 1.00 | 44.76 | 8 |
| | ATOM | 1708 | CB | ASP | A | 221 | 55.576 | 14.527 | -32.691 | 1.00 | 50.20 | 6 |
| | ATOM | 1709 | CG | ASP | A | 221 | 56.053 | 15.928 | -32.988 | 1.00 | 53.21 | 6 |
| | ATOM | 1710 | OD1 | ASP | A | 221 | 56.188 | 16.801 | -32.101 | 1.00 | 53.81 | 8 |
| | ATOM | 1711 | OD2 | ASP | A | 221 | 56.309 | 16.204 | -34.191 | 1.00 | 55.09 | 8 |
| 35 | ATOM | 1712 | N | LEU | A | 222 | 54.465 | 15.167 | -29.249 | 1.00 | 43.92 | 7 |
| | ATOM | 1713 | CA | LEU | A | 222 | 53.451 | 15.829 | -28.427 | 1.00 | 42.81 | 6 |
| | ATOM | 1714 | C | LEU | A | 222 | 53.215 | 17.271 | -28.774 | 1.00 | 43.64 | 6 |
| | ATOM | 1715 | O | LEU | A | 222 | 52.066 | 17.762 | -28.789 | 1.00 | 41.82 | 8 |
| | ATOM | 1716 | CB | LEU | A | 222 | 53.894 | 15.652 | -26.952 | 1.00 | 43.09 | 6 |
| 40 | ATOM | 1717 | CG | LEU | A | 222 | 54.196 | 14.191 | -26.578 | 1.00 | 41.83 | 6 |
| | ATOM | 1718 | CD1 | LEU | A | 222 | 54.442 | 14.033 | -25.081 | 1.00 | 42.53 | 6 |
| | ATOM | 1719 | CD2 | LEU | A | 222 | 53.086 | 13.237 | -26.991 | 1.00 | 41.15 | 6 |
| | ATOM | 1720 | N | ASP | A | 223 | 54.285 | 18.012 | -29.105 | 1.00 | 43.23 | 7 |
| | ATOM | 1721 | CA | ASP | A | 223 | 54.124 | 19.416 | -29.472 | 1.00 | 44.33 | 6 |
| 45 | ATOM | 1722 | C | ASP | A | 223 | 53.223 | 19.562 | -30.688 | 1.00 | 44.26 | 6 |
| | ATOM | 1723 | O | ASP | A | 223 | 52.401 | 20.490 | -30.770 | 1.00 | 45.10 | 8 |
| | ATOM | 1724 | CB | ASP | A | 223 | 55.508 | 20.042 | -29.717 | 1.00 | 45.77 | 6 |
| | ATOM | 1725 | N | GLU | A | 224 | 53.398 | 18.654 | -31.651 | 1.00 | 44.43 | 7 |
| | ATOM | 1726 | CA | GLU | A | 224 | 52.583 | 18.676 | -32.863 | 1.00 | 45.57 | 6 |
| 50 | ATOM | 1727 | C | GLU | A | 224 | 51.126 | 18.332 | -32.533 | 1.00 | 41.13 | 6 |
| | ATOM | 1728 | O | GLU | A | 224 | 50.187 | 18.995 | -32.967 | 1.00 | 40.57 | 8 |
| | ATOM | 1729 | CB | GLU | A | 224 | 53.146 | 17.723 | -33.915 | 1.00 | 49.14 | 6 |
| | ATOM | 1730 | CG | GLU | A | 224 | 52.327 | 17.645 | -35.186 | 1.00 | 53.71 | 6 |
| | ATOM | 1731 | CD | GLU | A | 224 | 52.241 | 18.926 | -35.991 | 1.00 | 57.27 | 6 |
| 55 | ATOM | 1732 | OE1 | GLU | A | 224 | 52.627 | 20.028 | -35.530 | 1.00 | 58.34 | 8 |
| | ATOM | 1733 | OE2 | GLU | A | 224 | 51.738 | 18.792 | -37.141 | 1.00 | 59.44 | 8 |
| | ATOM | 1734 | N | ILE | A | 225 | 50.928 | 17.234 | -31.837 | 1.00 | 38.07 | 7 |
| | ATOM | 1735 | CA | ILE | A | 225 | 49.602 | 16.821 | -31.360 | 1.00 | 36.44 | 6 |
| | ATOM | 1736 | C | ILE | A | 225 | 48.838 | 17.929 | -30.641 | 1.00 | 35.31 | 6 |
| 60 | ATOM | 1737 | O | ILE | A | 225 | 47.630 | 18.075 | -30.873 | 1.00 | 34.79 | 8 |
| | ATOM | 1738 | CB | ILE | A | 225 | 49.745 | 15.630 | -30.401 | 1.00 | 36.23 | 6 |
| | ATOM | 1739 | CG1 | ILE | A | 225 | 50.310 | 14.449 | -31.200 | 1.00 | 36.60 | 6 |
| | ATOM | 1740 | CG2 | ILE | A | 225 | 48.432 | 15.233 | -29.722 | 1.00 | 36.18 | 6 |
| | ATOM | 1741 | CD1 | ILE | A | 225 | 50.515 | 13.174 | -30.428 | 1.00 | 37.76 | 6 |
| 65 | ATOM | 1742 | N | ILE | A | 226 | 49.522 | 18.680 | -29.780 | 1.00 | 33.53 | 7 |
| | ATOM | 1743 | CA | ILE | A | 226 | 48.922 | 19.759 | -29.025 | 1.00 | 33.52 | 6 |
| | ATOM | 1744 | C | ILE | A | 226 | 48.614 | 20.969 | -29.881 | 1.00 | 33.80 | 6 |
| | ATOM | 1745 | O | ILE | A | 226 | 47.581 | 21.655 | -29.737 | 1.00 | 32.30 | 8 |
| | ATOM | 1746 | CB | ILE | A | 226 | 49.877 | 20.107 | -27.843 | 1.00 | 34.98 | 6 |
| 70 | ATOM | 1747 | CG1 | ILE | A | 226 | 49.847 | 18.937 | -26.874 | 1.00 | 34.99 | 6 |
| | ATOM | 1748 | CG2 | ILE | A | 226 | 49.490 | 21.417 | -27.159 | 1.00 | 34.94 | 6 |
| | ATOM | 1749 | CD1 | ILE | A | 226 | 50.657 | 19.117 | -25.611 | 1.00 | 36.97 | 6 |
| | ATOM | 1750 | N | THR | A | 227 | 49.527 | 21.261 | -30.830 | 1.00 | 33.69 | 7 |
| | ATOM | 1751 | CA | THR | A | 227 | 49.287 | 22.418 | -31.697 | 1.00 | 34.02 | 6 |
| | ATOM | 1752 | C | THR | A | 227 | 48.040 | 22.160 | -32.526 | 1.00 | 32.93 | 6 |

-60-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1753 | O | THR | A | 227 | 47.183 | 23.034 | -32.604 | 1.00 | 33.21 | 8 |
| | ATOM | 1754 | CB | THR | A | 227 | 50.469 | 22.754 | -32.630 | 1.00 | 36.23 | 6 |
| | ATOM | 1755 | OG1 | THR | A | 227 | 51.656 | 22.905 | -31.839 | 1.00 | 38.63 | 8 |
| 5 | ATOM | 1756 | CG2 | THR | A | 227 | 50.229 | 24.059 | -33.378 | 1.00 | 37.54 | 6 |
| | ATOM | 1757 | N | ILE | A | 228 | 47.887 | 20.967 | -33.060 | 1.00 | 33.57 | 7 |
| | ATOM | 1758 | CA | ILE | A | 228 | 46.742 | 20.647 | -33.899 | 1.00 | 33.85 | 6 |
| | ATOM | 1759 | C | ILE | A | 228 | 45.453 | 20.703 | -33.074 | 1.00 | 33.32 | 6 |
| | ATOM | 1760 | O | ILE | A | 228 | 44.417 | 21.205 | -33.482 | 1.00 | 31.47 | 8 |
| 10 | ATOM | 1761 | CB | ILE | A | 228 | 46.908 | 19.275 | -34.533 | 1.00 | 36.08 | 6 |
| | ATOM | 1762 | CG1 | ILE | A | 228 | 48.002 | 19.323 | -35.634 | 1.00 | 39.34 | 6 |
| | ATOM | 1763 | CG2 | ILE | A | 228 | 45.610 | 18.758 | -35.136 | 1.00 | 35.68 | 6 |
| | ATOM | 1764 | CD1 | ILE | A | 228 | 48.385 | 17.919 | -36.092 | 1.00 | 39.59 | 6 |
| | ATOM | 1765 | N | ALA | A | 229 | 45.597 | 20.146 | -31.859 | 1.00 | 33.09 | 7 |
| 15 | ATOM | 1766 | CA | ALA | A | 229 | 44.441 | 20.114 | -30.930 | 1.00 | 31.53 | 6 |
| | ATOM | 1767 | C | ALA | A | 229 | 43.948 | 21.497 | -30.607 | 1.00 | 28.89 | 6 |
| | ATOM | 1768 | O | ALA | A | 229 | 42.733 | 21.771 | -30.644 | 1.00 | 28.46 | 8 |
| | ATOM | 1769 | CB | ALA | A | 229 | 44.898 | 19.315 | -29.707 | 1.00 | 31.42 | 6 |
| | ATOM | 1770 | N | GLY | A | 230 | 44.836 | 22.471 | -30.407 | 1.00 | 29.20 | 7 |
| 20 | ATOM | 1771 | CA | GLY | A | 230 | 44.485 | 23.857 | -30.166 | 1.00 | 30.51 | 6 |
| | ATOM | 1772 | C | GLY | A | 230 | 43.797 | 24.472 | -31.372 | 1.00 | 31.48 | 6 |
| | ATOM | 1773 | O | GLY | A | 230 | 42.759 | 25.155 | -31.288 | 1.00 | 33.24 | 8 |
| | ATOM | 1774 | N | GLN | A | 231 | 44.374 | 24.217 | -32.569 | 1.00 | 33.19 | 7 |
| | ATOM | 1775 | CA | GLN | A | 231 | 43.812 | 24.700 | -33.823 | 1.00 | 33.48 | 6 |
| 25 | ATOM | 1776 | C | GLN | A | 231 | 42.396 | 24.206 | -34.027 | 1.00 | 32.96 | 6 |
| | ATOM | 1777 | O | GLN | A | 231 | 41.476 | 24.995 | -34.324 | 1.00 | 34.21 | 8 |
| | ATOM | 1778 | CB | GLN | A | 231 | 44.704 | 24.245 | -35.003 | 1.00 | 34.34 | 6 |
| | ATOM | 1779 | CG | GLN | A | 231 | 46.007 | 25.041 | -35.007 | 1.00 | 36.14 | 6 |
| | ATOM | 1780 | CD | GLN | A | 231 | 47.002 | 24.556 | -36.052 | 1.00 | 38.53 | 6 |
| 30 | ATOM | 1781 | OE1 | GLN | A | 231 | 46.812 | 23.541 | -36.732 | 1.00 | 39.14 | 8 |
| | ATOM | 1782 | NE2 | GLN | A | 231 | 48.085 | 25.312 | -36.189 | 1.00 | 39.12 | 7 |
| | ATOM | 1783 | N | GLU | A | 232 | 42.214 | 22.900 | -33.801 | 1.00 | 31.08 | 7 |
| | ATOM | 1784 | CA | GLU | A | 232 | 40.897 | 22.280 | -33.907 | 1.00 | 33.90 | 6 |
| | ATOM | 1785 | C | GLU | A | 232 | 39.897 | 22.898 | -32.923 | 1.00 | 32.79 | 6 |
| 35 | ATOM | 1786 | O | GLU | A | 232 | 38.785 | 23.235 | -33.345 | 1.00 | 30.71 | 8 |
| | ATOM | 1787 | CB | GLU | A | 232 | 40.956 | 20.772 | -33.659 | 1.00 | 36.16 | 6 |
| | ATOM | 1788 | CG | GLU | A | 232 | 41.681 | 19.963 | -34.705 | 1.00 | 40.99 | 6 |
| | ATOM | 1789 | CD | GLU | A | 232 | 41.956 | 18.526 | -34.336 | 1.00 | 43.88 | 6 |
| | ATOM | 1790 | OE1 | GLU | A | 232 | 42.231 | 18.222 | -33.162 | 1.00 | 46.75 | 8 |
| 40 | ATOM | 1791 | OE2 | GLU | A | 232 | 41.978 | 17.624 | -35.213 | 1.00 | 46.96 | 8 |
| | ATOM | 1792 | N | LEU | A | 233 | 40.279 | 23.075 | -31.654 | 1.00 | 31.79 | 7 |
| | ATOM | 1793 | CA | LEU | A | 233 | 39.390 | 23.738 | -30.717 | 1.00 | 31.75 | 6 |
| | ATOM | 1794 | C | LEU | A | 233 | 39.053 | 25.159 | -31.151 | 1.00 | 30.93 | 6 |
| | ATOM | 1795 | O | LEU | A | 233 | 37.914 | 25.617 | -31.117 | 1.00 | 29.58 | 8 |
| 45 | ATOM | 1796 | CB | LEU | A | 233 | 40.002 | 23.804 | -29.306 | 1.00 | 28.67 | 6 |
| | ATOM | 1797 | CG | LEU | A | 233 | 40.122 | 22.439 | -28.598 | 1.00 | 29.48 | 6 |
| | ATOM | 1798 | CD1 | LEU | A | 233 | 41.084 | 22.505 | -27.425 | 1.00 | 29.09 | 6 |
| | ATOM | 1799 | CD2 | LEU | A | 233 | 38.712 | 21.976 | -28.189 | 1.00 | 30.10 | 6 |
| | ATOM | 1800 | N | ASN | A | 234 | 40.083 | 25.889 | -31.615 | 1.00 | 32.79 | 7 |
| 50 | ATOM | 1801 | CA | ASN | A | 234 | 39.861 | 27.288 | -32.011 | 1.00 | 33.77 | 6 |
| | ATOM | 1802 | C | ASN | A | 234 | 38.946 | 27.388 | -33.220 | 1.00 | 31.44 | 6 |
| | ATOM | 1803 | O | ASN | A | 234 | 38.071 | 28.254 | -33.258 | 1.00 | 32.82 | 8 |
| | ATOM | 1804 | CB | ASN | A | 234 | 41.220 | 27.972 | -32.243 | 1.00 | 36.16 | 6 |
| | ATOM | 1805 | CG | ASN | A | 234 | 41.890 | 28.295 | -30.919 | 1.00 | 39.98 | 6 |
| 55 | ATOM | 1806 | OD1 | ASN | A | 234 | 41.296 | 28.257 | -29.838 | 1.00 | 40.76 | 8 |
| | ATOM | 1807 | ND2 | ASN | A | 234 | 43.185 | 28.592 | -30.922 | 1.00 | 39.55 | 7 |
| | ATOM | 1808 | N | GLU | A | 235 | 39.068 | 26.440 | -34.127 | 1.00 | 31.44 | 7 |
| | ATOM | 1809 | CA | GLU | A | 235 | 38.223 | 26.392 | -35.306 | 1.00 | 34.68 | 6 |
| | ATOM | 1810 | C | GLU | A | 235 | 36.779 | 26.082 | -34.971 | 1.00 | 34.35 | 6 |
| 60 | ATOM | 1811 | O | GLU | A | 235 | 35.878 | 26.565 | -35.629 | 1.00 | 35.56 | 8 |
| | ATOM | 1812 | CB | GLU | A | 235 | 38.763 | 25.314 | -36.244 | 1.00 | 36.35 | 6 |
| | ATOM | 1813 | N | LYS | A | 236 | 36.532 | 25.307 | -33.908 | 1.00 | 36.15 | 7 |
| | ATOM | 1814 | CA | LYS | A | 236 | 35.169 | 24.977 | -33.488 | 1.00 | 35.47 | 6 |
| | ATOM | 1815 | C | LYS | A | 236 | 34.483 | 26.106 | -32.738 | 1.00 | 34.87 | 6 |
| 65 | ATOM | 1816 | O | LYS | A | 236 | 33.253 | 26.085 | -32.561 | 1.00 | 36.38 | 8 |
| | ATOM | 1817 | CB | LYS | A | 236 | 35.213 | 23.748 | -32.577 | 1.00 | 37.47 | 6 |
| | ATOM | 1818 | CG | LYS | A | 236 | 35.609 | 22.450 | -33.245 | 1.00 | 38.51 | 6 |
| | ATOM | 1819 | CD | LYS | A | 236 | 35.643 | 21.345 | -32.192 | 1.00 | 40.94 | 6 |
| | ATOM | 1820 | CE | LYS | A | 236 | 36.184 | 20.083 | -32.827 | 1.00 | 42.93 | 6 |
| 70 | ATOM | 1821 | NZ | LYS | A | 236 | 36.231 | 18.973 | -31.850 | 1.00 | 45.15 | 7 |
| | ATOM | 1822 | N | GLY | A | 237 | 35.225 | 27.094 | -32.274 | 1.00 | 33.61 | 7 |
| | ATOM | 1823 | CA | GLY | A | 237 | 34.660 | 28.241 | -31.576 | 1.00 | 33.28 | 6 |
| | ATOM | 1824 | C | GLY | A | 237 | 35.127 | 28.401 | -30.157 | 1.00 | 32.89 | 6 |
| | ATOM | 1825 | O | GLY | A | 237 | 34.644 | 29.291 | -29.429 | 1.00 | 36.87 | 8 |
| | ATOM | 1826 | N | PHE | A | 238 | 36.017 | 27.546 | -29.668 | 1.00 | 30.90 | 7 |

-61-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1827 | CA | PHE | A | 238 | 36.629 | 27.664 | -28.380 | 1.00 | 31.61 | 6 |
| | ATOM | 1828 | C | PHE | A | 238 | 37.817 | 28.641 | -28.417 | 1.00 | 35.03 | 6 |
| | ATOM | 1829 | O | PHE | A | 238 | 38.191 | 29.022 | -29.528 | 1.00 | 37.95 | 8 |
| 5 | ATOM | 1830 | CB | PHE | A | 238 | 37.201 | 26.338 | -27.875 | 1.00 | 29.76 | 6 |
| | ATOM | 1831 | CG | PHE | A | 238 | 36.165 | 25.258 | -27.686 | 1.00 | 30.50 | 6 |
| | ATOM | 1832 | CD1 | PHE | A | 238 | 35.712 | 24.500 | -28.727 | 1.00 | 29.47 | 6 |
| | ATOM | 1833 | CD2 | PHE | A | 238 | 35.679 | 24.979 | -26.414 | 1.00 | 31.42 | 6 |
| | ATOM | 1834 | CE1 | PHE | A | 238 | 34.752 | 23.501 | -28.555 | 1.00 | 31.11 | 6 |
| 10 | ATOM | 1835 | CE2 | PHE | A | 238 | 34.731 | 23.986 | -26.233 | 1.00 | 29.77 | 6 |
| | ATOM | 1836 | CZ | PHE | A | 238 | 34.284 | 23.235 | -27.279 | 1.00 | 29.29 | 6 |
| | ATOM | 1837 | N | ARG | A | 239 | 38.388 | 28.963 | -27.268 | 1.00 | 34.76 | 7 |
| | ATOM | 1838 | CA | ARG | A | 239 | 39.674 | 29.645 | -27.216 | 1.00 | 35.49 | 6 |
| | ATOM | 1839 | C | ARG | A | 239 | 40.472 | 28.742 | -26.270 | 1.00 | 35.32 | 6 |
| 15 | ATOM | 1840 | O | ARG | A | 239 | 40.308 | 28.724 | -25.057 | 1.00 | 32.89 | 8 |
| | ATOM | 1841 | CB | ARG | A | 239 | 39.721 | 31.088 | -26.754 | 1.00 | 37.36 | 6 |
| | ATOM | 1842 | CG | ARG | A | 239 | 39.226 | 32.068 | -27.822 | 1.00 | 39.64 | 6 |
| | ATOM | 1843 | N | ALA | A | 240 | 41.233 | 27.877 | -26.931 | 1.00 | 36.31 | 7 |
| | ATOM | 1844 | CA | ALA | A | 240 | 42.124 | 26.921 | -26.293 | 1.00 | 36.79 | 6 |
| 20 | ATOM | 1845 | C | ALA | A | 240 | 42.906 | 27.617 | -25.203 | 1.00 | 38.54 | 6 |
| | ATOM | 1846 | O | ALA | A | 240 | 43.360 | 28.735 | -25.495 | 1.00 | 39.25 | 8 |
| | ATOM | 1847 | CB | ALA | A | 240 | 43.087 | 26.347 | -27.333 | 1.00 | 36.86 | 6 |
| | ATOM | 1848 | N | ASP | A | 241 | 43.035 | 27.053 | -24.024 | 1.00 | 39.01 | 7 |
| | ATOM | 1849 | CA | ASP | A | 241 | 43.689 | 27.789 | -22.947 | 1.00 | 42.42 | 6 |
| 25 | ATOM | 1850 | C | ASP | A | 241 | 44.867 | 27.010 | -22.396 | 1.00 | 43.73 | 6 |
| | ATOM | 1851 | O | ASP | A | 241 | 45.894 | 27.608 | -22.061 | 1.00 | 46.19 | 8 |
| | ATOM | 1852 | CB | ASP | A | 241 | 42.686 | 28.105 | -21.828 | 1.00 | 43.72 | 6 |
| | ATOM | 1853 | CG | ASP | A | 241 | 43.319 | 28.991 | -20.771 | 1.00 | 46.29 | 6 |
| | ATOM | 1854 | OD1 | ASP | A | 241 | 43.712 | 30.124 | -21.130 | 1.00 | 47.38 | 8 |
| 30 | ATOM | 1855 | OD2 | ASP | A | 241 | 43.433 | 28.560 | -19.610 | 1.00 | 46.21 | 8 |
| | ATOM | 1856 | N | ASP | A | 242 | 44.733 | 25.690 | -22.292 | 1.00 | 41.53 | 7 |
| | ATOM | 1857 | CA | ASP | A | 242 | 45.828 | 24.876 | -21.764 | 1.00 | 39.46 | 6 |
| | ATOM | 1858 | C | ASP | A | 242 | 45.607 | 23.442 | -22.177 | 1.00 | 37.10 | 6 |
| | ATOM | 1859 | O | ASP | A | 242 | 44.496 | 22.895 | -22.059 | 1.00 | 34.02 | 8 |
| 35 | ATOM | 1860 | CB | ASP | A | 242 | 45.908 | 25.001 | -20.242 | 1.00 | 43.32 | 6 |
| | ATOM | 1861 | CG | ASP | A | 242 | 47.103 | 24.275 | -19.661 | 1.00 | 47.37 | 6 |
| | ATOM | 1862 | OD1 | ASP | A | 242 | 46.980 | 23.437 | -18.736 | 1.00 | 49.59 | 8 |
| | ATOM | 1863 | OD2 | ASP | A | 242 | 48.231 | 24.530 | -20.158 | 1.00 | 50.50 | 8 |
| 40 | ATOM | 1864 | N | ILE | A | 243 | 46.597 | 22.785 | -22.750 | 1.00 | 33.48 | 7 |
| | ATOM | 1865 | CA | ILE | A | 243 | 46.550 | 21.419 | -23.193 | 1.00 | 32.08 | 6 |
| | ATOM | 1866 | C | ILE | A | 243 | 47.853 | 20.812 | -22.718 | 1.00 | 33.41 | 6 |
| | ATOM | 1867 | O | ILE | A | 243 | 48.895 | 21.390 | -23.062 | 1.00 | 32.28 | 8 |
| | ATOM | 1868 | CB | ILE | A | 243 | 46.424 | 21.205 | -24.719 | 1.00 | 33.19 | 6 |
| | ATOM | 1869 | CG1 | ILE | A | 243 | 45.141 | 21.847 | -25.222 | 1.00 | 33.31 | 6 |
| 45 | ATOM | 1870 | CG2 | ILE | A | 243 | 46.504 | 19.703 | -24.995 | 1.00 | 32.88 | 6 |
| | ATOM | 1871 | CD1 | ILE | A | 243 | 44.892 | 21.792 | -26.713 | 1.00 | 33.52 | 6 |
| | ATOM | 1872 | N | GLN | A | 244 | 47.829 | 19.735 | -21.975 | 1.00 | 33.31 | 7 |
| | ATOM | 1873 | CA | GLN | A | 244 | 49.003 | 19.097 | -21.436 | 1.00 | 35.24 | 6 |
| | ATOM | 1874 | C | GLN | A | 244 | 48.849 | 17.592 | -21.483 | 1.00 | 34.74 | 6 |
| 50 | ATOM | 1875 | O | GLN | A | 244 | 47.741 | 17.056 | -21.422 | 1.00 | 33.25 | 8 |
| | ATOM | 1876 | CB | GLN | A | 244 | 49.300 | 19.528 | -19.967 | 1.00 | 39.02 | 6 |
| | ATOM | 1877 | CG | GLN | A | 244 | 49.773 | 20.962 | -19.905 | 1.00 | 43.89 | 6 |
| | ATOM | 1878 | CD | GLN | A | 244 | 50.076 | 21.564 | -18.569 | 1.00 | 47.28 | 6 |
| | ATOM | 1879 | OE1 | GLN | A | 244 | 50.148 | 20.870 | -17.548 | 1.00 | 48.52 | 8 |
| 55 | ATOM | 1880 | NE2 | GLN | A | 244 | 50.259 | 22.895 | -18.597 | 1.00 | 49.46 | 7 |
| | ATOM | 1881 | N | ILE | A | 245 | 49.943 | 16.870 | -21.716 | 1.00 | 31.86 | 7 |
| | ATOM | 1882 | CA | ILE | A | 245 | 50.000 | 15.439 | -21.801 | 1.00 | 31.75 | 6 |
| | ATOM | 1883 | C | ILE | A | 245 | 51.110 | 14.967 | -20.852 | 1.00 | 33.59 | 6 |
| | ATOM | 1884 | O | ILE | A | 245 | 52.183 | 15.586 | -20.888 | 1.00 | 36.14 | 8 |
| 60 | ATOM | 1885 | CB | ILE | A | 245 | 50.299 | 14.888 | -23.213 | 1.00 | 33.28 | 6 |
| | ATOM | 1886 | CG1 | ILE | A | 245 | 49.188 | 15.324 | -24.177 | 1.00 | 32.78 | 6 |
| | ATOM | 1887 | CG2 | ILE | A | 245 | 50.470 | 13.387 | -23.164 | 1.00 | 33.13 | 6 |
| | ATOM | 1888 | CD1 | ILE | A | 245 | 49.424 | 15.049 | -25.648 | 1.00 | 33.13 | 6 |
| | ATOM | 1889 | N | ARG | A | 246 | 50.827 | 14.054 | -19.946 | 1.00 | 34.84 | 7 |
| 65 | ATOM | 1890 | CA | ARG | A | 246 | 51.816 | 13.609 | -18.982 | 1.00 | 35.92 | 6 |
| | ATOM | 1891 | C | ARG | A | 246 | 51.687 | 12.122 | -18.690 | 1.00 | 35.36 | 6 |
| | ATOM | 1892 | O | ARG | A | 246 | 50.697 | 11.461 | -18.911 | 1.00 | 35.88 | 8 |
| | ATOM | 1893 | CB | ARG | A | 246 | 51.713 | 14.251 | -17.589 | 1.00 | 36.79 | 6 |
| | ATOM | 1894 | CG | ARG | A | 246 | 51.674 | 15.747 | -17.458 | 1.00 | 41.24 | 6 |
| 70 | ATOM | 1895 | CD | ARG | A | 246 | 53.032 | 16.284 | -17.914 | 1.00 | 46.18 | 6 |
| | ATOM | 1896 | NE | ARG | A | 246 | 53.251 | 17.654 | -17.502 | 1.00 | 49.48 | 7 |
| | ATOM | 1897 | CZ | ARG | A | 246 | 53.913 | 18.040 | -16.420 | 1.00 | 51.58 | 6 |
| | ATOM | 1898 | NH1 | ARG | A | 246 | 54.466 | 17.155 | -15.603 | 1.00 | 51.91 | 7 |
| | ATOM | 1899 | NH2 | ARG | A | 246 | 54.006 | 19.352 | -16.229 | 1.00 | 53.89 | 7 |
| | ATOM | 1900 | N | ASP | A | 247 | 52.730 | 11.616 | -18.003 | 1.00 | 35.81 | 7 |

-62-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1901 | CA | ASP | A | 247 | 52.753 | 10.248 | -17.537 | 1.00 | 34.88 | 6 |
| | ATOM | 1902 | C | ASP | A | 247 | 51.652 | 10.087 | -16.495 | 1.00 | 31.75 | 6 |
| | ATOM | 1903 | O | ASP | A | 247 | 51.690 | 10.908 | -15.584 | 1.00 | 32.95 | 8 |
| 5 | ATOM | 1904 | CB | ASP | A | 247 | 54.146 | 9.952 | -16.954 | 1.00 | 37.68 | 6 |
| | ATOM | 1905 | CG | ASP | A | 247 | 54.195 | 8.479 | -16.611 | 1.00 | 39.66 | 6 |
| | ATOM | 1906 | OD1 | ASP | A | 247 | 53.482 | 8.015 | -15.710 | 1.00 | 41.79 | 8 |
| | ATOM | 1907 | OD2 | ASP | A | 247 | 54.924 | 7.748 | -17.284 | 1.00 | 42.94 | 8 |
| | ATOM | 1908 | N | ALA | A | 248 | 50.712 | 9.185 | -16.600 | 1.00 | 33.81 | 7 |
| 10 | ATOM | 1909 | CA | ALA | A | 248 | 49.616 | 9.156 | -15.609 | 1.00 | 32.51 | 6 |
| | ATOM | 1910 | C | ALA | A | 248 | 50.041 | 8.675 | -14.232 | 1.00 | 34.35 | 6 |
| | ATOM | 1911 | O | ALA | A | 248 | 49.399 | 9.063 | -13.249 | 1.00 | 33.85 | 8 |
| | ATOM | 1912 | CB | ALA | A | 248 | 48.499 | 8.253 | -16.070 | 1.00 | 33.01 | 6 |
| | ATOM | 1913 | N | ASP | A | 249 | 51.057 | 7.825 | -14.103 | 1.00 | 36.10 | 7 |
| 15 | ATOM | 1914 | CA | ASP | A | 249 | 51.462 | 7.281 | -12.822 | 1.00 | 35.70 | 6 |
| | ATOM | 1915 | C | ASP | A | 249 | 52.421 | 8.185 | -12.073 | 1.00 | 33.40 | 6 |
| | ATOM | 1916 | O | ASP | A | 249 | 52.399 | 8.230 | -10.818 | 1.00 | 31.30 | 8 |
| | ATOM | 1917 | CB | ASP | A | 249 | 52.152 | 5.916 | -13.031 | 1.00 | 39.11 | 6 |
| | ATOM | 1918 | CG | ASP | A | 249 | 51.137 | 5.007 | -13.715 | 1.00 | 43.20 | 6 |
| 20 | ATOM | 1919 | OD1 | ASP | A | 249 | 50.028 | 4.826 | -13.134 | 1.00 | 45.31 | 8 |
| | ATOM | 1920 | OD2 | ASP | A | 249 | 51.423 | 4.514 | -14.817 | 1.00 | 43.99 | 8 |
| | ATOM | 1921 | N | THR | A | 250 | 53.275 | 8.844 | -12.857 | 1.00 | 31.16 | 7 |
| | ATOM | 1922 | CA | THR | A | 250 | 54.301 | 9.667 | -12.240 | 1.00 | 32.87 | 6 |
| | ATOM | 1923 | C | THR | A | 250 | 54.087 | 11.144 | -12.416 | 1.00 | 32.81 | 6 |
| 25 | ATOM | 1924 | O | THR | A | 250 | 54.760 | 11.935 | -11.789 | 1.00 | 30.56 | 8 |
| | ATOM | 1925 | CB | THR | A | 250 | 55.740 | 9.378 | -12.792 | 1.00 | 34.12 | 6 |
| | ATOM | 1926 | OG1 | THR | A | 250 | 55.779 | 9.795 | -14.158 | 1.00 | 34.42 | 8 |
| | ATOM | 1927 | CG2 | THR | A | 250 | 56.080 | 7.911 | -12.637 | 1.00 | 34.28 | 6 |
| | ATOM | 1928 | N | LEU | A | 251 | 53.281 | 11.587 | -13.365 | 1.00 | 32.56 | 7 |
| 30 | ATOM | 1929 | CA | LEU | A | 251 | 52.972 | 12.978 | -13.672 | 1.00 | 34.35 | 6 |
| | ATOM | 1930 | C | LEU | A | 251 | 54.124 | 13.689 | -14.360 | 1.00 | 35.41 | 6 |
| | ATOM | 1931 | O | LEU | A | 251 | 54.093 | 14.893 | -14.592 | 1.00 | 35.99 | 8 |
| | ATOM | 1932 | CB | LEU | A | 251 | 52.494 | 13.758 | -12.418 | 1.00 | 33.68 | 6 |
| | ATOM | 1933 | CG | LEU | A | 251 | 51.220 | 13.147 | -11.792 | 1.00 | 34.55 | 6 |
| 35 | ATOM | 1934 | CD1 | LEU | A | 251 | 50.797 | 13.969 | -10.573 | 1.00 | 35.91 | 6 |
| | ATOM | 1935 | CD2 | LEU | A | 251 | 50.101 | 13.012 | -12.821 | 1.00 | 35.43 | 6 |
| | ATOM | 1936 | N | LEU | A | 252 | 55.194 | 12.962 | -14.695 | 1.00 | 39.58 | 7 |
| | ATOM | 1937 | CA | LEU | A | 252 | 56.323 | 13.507 | -15.418 | 1.00 | 40.96 | 6 |
| | ATOM | 1938 | C | LEU | A | 252 | 55.945 | 13.614 | -16.874 | 1.00 | 43.27 | 6 |
| 40 | ATOM | 1939 | O | LEU | A | 252 | 54.906 | 13.129 | -17.318 | 1.00 | 40.97 | 8 |
| | ATOM | 1940 | CB | LEU | A | 252 | 57.550 | 12.584 | -15.264 | 1.00 | 42.55 | 6 |
| | ATOM | 1941 | CG | LEU | A | 252 | 58.072 | 12.496 | -13.823 | 1.00 | 43.46 | 6 |
| | ATOM | 1942 | CD1 | LEU | A | 252 | 59.196 | 11.476 | -13.685 | 1.00 | 44.26 | 6 |
| | ATOM | 1943 | CD2 | LEU | A | 252 | 58.546 | 13.868 | -13.341 | 1.00 | 43.34 | 6 |
| 45 | ATOM | 1944 | N | GLU | A | 253 | 56.855 | 14.189 | -17.659 | 1.00 | 46.27 | 7 |
| | ATOM | 1945 | CA | GLU | A | 253 | 56.716 | 14.144 | -19.109 | 1.00 | 48.94 | 6 |
| | ATOM | 1946 | C | GLU | A | 253 | 56.642 | 12.706 | -19.612 | 1.00 | 48.01 | 6 |
| | ATOM | 1947 | O | GLU | A | 253 | 57.291 | 11.928 | -18.871 | 1.00 | 48.08 | 8 |
| | ATOM | 1948 | CB | GLU | A | 253 | 57.877 | 14.878 | -19.783 | 1.00 | 52.86 | 6 |
| 50 | ATOM | 1949 | CG | GLU | A | 253 | 57.914 | 16.371 | -19.500 | 1.00 | 57.25 | 6 |
| | ATOM | 1950 | CD | GLU | A | 253 | 56.720 | 17.104 | -20.077 | 1.00 | 60.45 | 6 |
| | ATOM | 1951 | OE1 | GLU | A | 253 | 56.308 | 16.771 | -21.207 | 1.00 | 61.73 | 8 |
| | ATOM | 1952 | OE2 | GLU | A | 253 | 56.194 | 18.011 | -19.397 | 1.00 | 61.77 | 8 |
| | ATOM | 1953 | N | VAL | A | 254 | 55.835 | 12.324 | -20.596 | 1.00 | 48.66 | 7 |
| 55 | ATOM | 1954 | CA | VAL | A | 254 | 55.849 | 10.887 | -20.872 | 1.00 | 49.85 | 6 |
| | ATOM | 1955 | C | VAL | A | 254 | 57.149 | 10.638 | -21.614 | 1.00 | 51.30 | 6 |
| | ATOM | 1956 | O | VAL | A | 254 | 57.658 | 11.494 | -22.340 | 1.00 | 49.27 | 8 |
| | ATOM | 1957 | CB | VAL | A | 254 | 54.576 | 10.399 | -21.614 | 1.00 | 51.06 | 6 |
| | ATOM | 1958 | CG1 | VAL | A | 254 | 53.600 | 11.541 | -21.825 | 1.00 | 50.21 | 6 |
| 60 | ATOM | 1959 | CG2 | VAL | A | 254 | 54.935 | 9.757 | -22.940 | 1.00 | 51.39 | 6 |
| | ATOM | 1960 | N | SER | A | 255 | 57.636 | 9.432 | -21.398 | 1.00 | 50.78 | 7 |
| | ATOM | 1961 | CA | SER | A | 255 | 58.878 | 8.951 | -21.946 | 1.00 | 52.29 | 6 |
| | ATOM | 1962 | C | SER | A | 255 | 58.718 | 7.516 | -22.423 | 1.00 | 53.07 | 6 |
| | ATOM | 1963 | O | SER | A | 255 | 57.625 | 6.965 | -22.444 | 1.00 | 53.08 | 8 |
| 65 | ATOM | 1964 | CB | SER | A | 255 | 59.978 | 8.985 | -20.878 | 1.00 | 51.99 | 6 |
| | ATOM | 1965 | OG | SER | A | 255 | 59.761 | 7.859 | -20.013 | 1.00 | 51.83 | 8 |
| | ATOM | 1966 | N | GLU | A | 256 | 59.844 | 6.858 | -22.692 | 1.00 | 55.01 | 7 |
| | ATOM | 1967 | CA | GLU | A | 256 | 59.903 | 5.485 | -23.155 | 1.00 | 55.63 | 6 |
| | ATOM | 1968 | C | GLU | A | 256 | 59.251 | 4.493 | -22.207 | 1.00 | 55.82 | 6 |
| 70 | ATOM | 1969 | O | GLU | A | 256 | 58.566 | 3.543 | -22.591 | 1.00 | 55.91 | 8 |
| | ATOM | 1970 | CB | GLU | A | 256 | 61.380 | 5.091 | -23.350 | 1.00 | 56.43 | 6 |
| | ATOM | 1971 | N | THR | A | 257 | 59.458 | 4.732 | -20.919 | 1.00 | 55.14 | 7 |
| | ATOM | 1972 | CA | THR | A | 257 | 58.921 | 3.928 | -19.846 | 1.00 | 54.05 | 6 |
| | ATOM | 1973 | C | THR | A | 257 | 57.443 | 4.151 | -19.554 | 1.00 | 51.69 | 6 |
| | ATOM | 1974 | O | THR | A | 257 | 56.836 | 3.301 | -18.887 | 1.00 | 51.58 | 8 |

-63-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 1975 | CB | THR | A | 257 | 59.723 | 4.223 | -18.554 | 1.00 | 55.07 | 6 |
| | ATOM | 1976 | OG1 | THR | A | 257 | 59.404 | 5.533 | -18.065 | 1.00 | 56.77 | 8 |
| | ATOM | 1977 | CG2 | THR | A | 257 | 61.215 | 4.150 | -18.828 | 1.00 | 55.65 | 6 |
| 5 | ATOM | 1978 | N | SER | A | 258 | 56.834 | 5.252 | -20.000 | 1.00 | 49.85 | 7 |
| | ATOM | 1979 | CA | SER | A | 258 | 55.426 | 5.481 | -19.663 | 1.00 | 46.23 | 6 |
| | ATOM | 1980 | C | SER | A | 258 | 54.484 | 4.382 | -20.104 | 1.00 | 46.46 | 6 |
| | ATOM | 1981 | O | SER | A | 258 | 54.511 | 3.984 | -21.269 | 1.00 | 47.83 | 8 |
| | ATOM | 1982 | CB | SER | A | 258 | 54.950 | 6.783 | -20.306 | 1.00 | 44.06 | 6 |
| 10 | ATOM | 1983 | OG | SER | A | 258 | 55.742 | 7.841 | -19.839 | 1.00 | 40.94 | 8 |
| | ATOM | 1984 | N | LYS | A | 259 | 53.626 | 3.905 | -19.221 | 1.00 | 46.05 | 7 |
| | ATOM | 1985 | CA | LYS | A | 259 | 52.624 | 2.902 | -19.512 | 1.00 | 46.69 | 6 |
| | ATOM | 1986 | C | LYS | A | 259 | 51.252 | 3.551 | -19.739 | 1.00 | 45.85 | 6 |
| | ATOM | 1987 | O | LYS | A | 259 | 50.329 | 3.046 | -20.369 | 1.00 | 45.29 | 8 |
| 15 | ATOM | 1988 | CB | LYS | A | 259 | 52.455 | 1.886 | -18.382 | 1.00 | 46.44 | 6 |
| | ATOM | 1989 | CG | LYS | A | 259 | 53.726 | 1.200 | -17.920 | 1.00 | 47.93 | 6 |
| | ATOM | 1990 | N | ARG | A | 260 | 51.088 | 4.696 | -19.069 | 1.00 | 46.77 | 7 |
| | ATOM | 1991 | CA | ARG | A | 260 | 49.800 | 5.397 | -19.104 | 1.00 | 45.39 | 6 |
| | ATOM | 1992 | C | ARG | A | 260 | 49.991 | 6.882 | -19.278 | 1.00 | 41.75 | 6 |
| 20 | ATOM | 1993 | O | ARG | A | 260 | 50.970 | 7.421 | -18.763 | 1.00 | 41.96 | 8 |
| | ATOM | 1994 | CB | ARG | A | 260 | 49.004 | 5.146 | -17.814 | 1.00 | 48.72 | 6 |
| | ATOM | 1995 | CG | ARG | A | 260 | 48.340 | 3.797 | -17.715 | 1.00 | 52.78 | 6 |
| | ATOM | 1996 | CD | ARG | A | 260 | 47.783 | 3.490 | -16.342 | 1.00 | 56.11 | 6 |
| | ATOM | 1997 | NE | ARG | A | 260 | 48.800 | 3.016 | -15.423 | 1.00 | 60.02 | 7 |
| 25 | ATOM | 1998 | CZ | ARG | A | 260 | 49.366 | 1.817 | -15.362 | 1.00 | 61.86 | 6 |
| | ATOM | 1999 | NH1 | ARG | A | 260 | 49.066 | 0.806 | -16.179 | 1.00 | 62.97 | 7 |
| | ATOM | 2000 | NH2 | ARG | A | 260 | 50.275 | 1.615 | -14.410 | 1.00 | 62.19 | 7 |
| | ATOM | 2001 | N | ALA | A | 261 | 49.079 | 7.547 | -20.024 | 1.00 | 39.42 | 7 |
| | ATOM | 2002 | CA | ALA | A | 261 | 49.232 | 8.993 | -20.107 | 1.00 | 35.31 | 6 |
| 30 | ATOM | 2003 | C | ALA | A | 261 | 47.928 | 9.630 | -19.612 | 1.00 | 32.26 | 6 |
| | ATOM | 2004 | O | ALA | A | 261 | 46.872 | 9.005 | -19.790 | 1.00 | 34.66 | 8 |
| | ATOM | 2005 | CB | ALA | A | 261 | 49.538 | 9.504 | -21.504 | 1.00 | 34.95 | 6 |
| | ATOM | 2006 | N | VAL | A | 262 | 48.060 | 10.831 | -19.087 | 1.00 | 29.67 | 7 |
| | ATOM | 2007 | CA | VAL | A | 262 | 46.852 | 11.578 | -18.705 | 1.00 | 27.51 | 6 |
| 35 | ATOM | 2008 | C | VAL | A | 262 | 46.916 | 12.796 | -19.608 | 1.00 | 27.97 | 6 |
| | ATOM | 2009 | O | VAL | A | 262 | 47.977 | 13.414 | -19.791 | 1.00 | 26.28 | 8 |
| | ATOM | 2010 | CB | VAL | A | 262 | 46.750 | 11.979 | -17.233 | 1.00 | 29.25 | 6 |
| | ATOM | 2011 | CG1 | VAL | A | 262 | 47.995 | 12.725 | -16.785 | 1.00 | 30.58 | 6 |
| | ATOM | 2012 | CG2 | VAL | A | 262 | 45.527 | 12.884 | -16.976 | 1.00 | 30.36 | 6 |
| 40 | ATOM | 2013 | N | ILE | A | 263 | 45.801 | 13.185 | -20.185 | 1.00 | 26.21 | 7 |
| | ATOM | 2014 | CA | ILE | A | 263 | 45.639 | 14.343 | -21.031 | 1.00 | 26.33 | 6 |
| | ATOM | 2015 | C | ILE | A | 263 | 44.738 | 15.341 | -20.300 | 1.00 | 28.09 | 6 |
| | ATOM | 2016 | O | ILE | A | 263 | 43.635 | 14.903 | -19.935 | 1.00 | 26.14 | 8 |
| | ATOM | 2017 | CB | ILE | A | 263 | 44.977 | 13.970 | -22.357 | 1.00 | 27.18 | 6 |
| 45 | ATOM | 2018 | CG1 | ILE | A | 263 | 45.701 | 12.767 | -22.999 | 1.00 | 30.42 | 6 |
| | ATOM | 2019 | CG2 | ILE | A | 263 | 44.931 | 15.184 | -23.302 | 1.00 | 26.41 | 6 |
| | ATOM | 2020 | CD1 | ILE | A | 263 | 44.751 | 11.943 | -23.867 | 1.00 | 32.55 | 6 |
| | ATOM | 2021 | N | LEU | A | 264 | 45.198 | 16.564 | -20.149 | 1.00 | 28.73 | 7 |
| | ATOM | 2022 | CA | LEU | A | 264 | 44.453 | 17.626 | -19.514 | 1.00 | 30.58 | 6 |
| 50 | ATOM | 2023 | C | LEU | A | 264 | 44.108 | 18.698 | -20.530 | 1.00 | 29.44 | 6 |
| | ATOM | 2024 | O | LEU | A | 264 | 45.005 | 19.177 | -21.235 | 1.00 | 30.50 | 8 |
| | ATOM | 2025 | CB | LEU | A | 264 | 45.273 | 18.264 | -18.392 | 1.00 | 33.45 | 6 |
| | ATOM | 2026 | CG | LEU | A | 264 | 46.310 | 17.397 | -17.677 | 1.00 | 35.36 | 6 |
| | ATOM | 2027 | CD1 | LEU | A | 264 | 47.287 | 18.261 | -16.855 | 1.00 | 38.43 | 6 |
| 55 | ATOM | 2028 | CD2 | LEU | A | 264 | 45.634 | 16.357 | -16.800 | 1.00 | 36.22 | 6 |
| | ATOM | 2029 | N | VAL | A | 265 | 42.875 | 19.166 | -20.643 | 1.00 | 28.12 | 7 |
| | ATOM | 2030 | CA | VAL | A | 265 | 42.516 | 20.228 | -21.586 | 1.00 | 30.77 | 6 |
| | ATOM | 2031 | C | VAL | A | 265 | 41.662 | 21.288 | -20.868 | 1.00 | 30.38 | 6 |
| | ATOM | 2032 | O | VAL | A | 265 | 40.888 | 20.946 | -19.964 | 1.00 | 33.23 | 8 |
| 60 | ATOM | 2033 | CB | VAL | A | 265 | 41.740 | 19.716 | -22.798 | 1.00 | 30.45 | 6 |
| | ATOM | 2034 | CG1 | VAL | A | 265 | 42.546 | 18.732 | -23.649 | 1.00 | 31.64 | 6 |
| | ATOM | 2035 | CG2 | VAL | A | 265 | 40.456 | 18.962 | -22.415 | 1.00 | 30.65 | 6 |
| | ATOM | 2036 | N | ALA | A | 266 | 41.822 | 22.538 | -21.233 | 1.00 | 30.29 | 7 |
| | ATOM | 2037 | CA | ALA | A | 266 | 40.992 | 23.628 | -20.697 | 1.00 | 27.93 | 6 |
| 65 | ATOM | 2038 | C | ALA | A | 266 | 40.722 | 24.514 | -21.890 | 1.00 | 28.75 | 6 |
| | ATOM | 2039 | O | ALA | A | 266 | 41.687 | 24.771 | -22.653 | 1.00 | 31.65 | 8 |
| | ATOM | 2040 | CB | ALA | A | 266 | 41.637 | 24.388 | -19.574 | 1.00 | 28.93 | 6 |
| | ATOM | 2041 | N | ALA | A | 267 | 39.535 | 25.012 | -22.069 | 1.00 | 27.14 | 7 |
| | ATOM | 2042 | CA | ALA | A | 267 | 39.237 | 25.880 | -23.189 | 1.00 | 28.13 | 6 |
| 70 | ATOM | 2043 | C | ALA | A | 267 | 38.051 | 26.744 | -22.796 | 1.00 | 29.67 | 6 |
| | ATOM | 2044 | O | ALA | A | 267 | 37.054 | 26.257 | -22.261 | 1.00 | 27.60 | 8 |
| | ATOM | 2045 | CB | ALA | A | 267 | 38.861 | 25.167 | -24.478 | 1.00 | 26.05 | 6 |
| | ATOM | 2046 | N | TRP | A | 268 | 38.151 | 28.007 | -23.166 | 1.00 | 29.63 | 7 |
| | ATOM | 2047 | CA | TRP | A | 268 | 37.074 | 28.951 | -22.969 | 1.00 | 28.26 | 6 |
| | ATOM | 2048 | C | TRP | A | 268 | 36.049 | 28.766 | -24.072 | 1.00 | 29.88 | 6 |

-64-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|---|
| | ATOM | 2049 | O | TRP | A | 268 | 36.407 | 28.609 | -25.245 | 1.00 | 30.20 | 8 |
| | ATOM | 2050 | CB | TRP | A | 268 | 37.599 | 30.394 | -22.996 | 1.00 | 30.40 | 6 |
| | ATOM | 2051 | CG | TRP | A | 268 | 38.406 | 30.735 | -21.778 | 1.00 | 31.50 | 6 |
| 5 | ATOM | 2052 | CD1 | TRP | A | 268 | 39.756 | 30.638 | -21.572 | 1.00 | 32.04 | 6 |
| | ATOM | 2053 | CD2 | TRP | A | 268 | 37.850 | 31.336 | -20.602 | 1.00 | 29.94 | 6 |
| | ATOM | 2054 | NE1 | TRP | A | 268 | 40.071 | 31.097 | -20.307 | 1.00 | 32.09 | 7 |
| | ATOM | 2055 | CE2 | TRP | A | 268 | 38.905 | 31.521 | -19.699 | 1.00 | 32.20 | 6 |
| | ATOM | 2056 | CE3 | TRP | A | 268 | 36.543 | 31.660 | -20.214 | 1.00 | 29.41 | 6 |
| 10 | ATOM | 2057 | CZ2 | TRP | A | 268 | 38.729 | 32.062 | -18.420 | 1.00 | 30.97 | 6 |
| | ATOM | 2058 | CZ3 | TRP | A | 268 | 36.362 | 32.188 | -18.965 | 1.00 | 30.37 | 6 |
| | ATOM | 2059 | CH2 | TRP | A | 268 | 37.448 | 32.390 | -18.097 | 1.00 | 29.74 | 6 |
| | ATOM | 2060 | N | LEU | A | 269 | 34.789 | 28.947 | -23.715 | 1.00 | 28.17 | 7 |
| | ATOM | 2061 | CA | LEU | A | 269 | 33.648 | 28.954 | -24.579 | 1.00 | 29.03 | 6 |
| 15 | ATOM | 2062 | C | LEU | A | 269 | 32.680 | 29.913 | -23.885 | 1.00 | 29.91 | 6 |
| | ATOM | 2063 | O | LEU | A | 269 | 32.201 | 29.674 | -22.758 | 1.00 | 25.57 | 8 |
| | ATOM | 2064 | CB | LEU | A | 269 | 33.139 | 27.528 | -24.786 | 1.00 | 30.48 | 6 |
| | ATOM | 2065 | CG | LEU | A | 269 | 31.952 | 27.443 | -25.719 | 1.00 | 31.96 | 6 |
| | ATOM | 2066 | CD1 | LEU | A | 269 | 32.337 | 27.993 | -27.103 | 1.00 | 30.89 | 6 |
| 20 | ATOM | 2067 | CD2 | LEU | A | 269 | 31.423 | 26.003 | -25.790 | 1.00 | 31.19 | 6 |
| | ATOM | 2068 | N | GLY | A | 270 | 32.559 | 31.132 | -24.446 | 1.00 | 29.19 | 7 |
| | ATOM | 2069 | CA | GLY | A | 270 | 31.738 | 32.156 | -23.798 | 1.00 | 29.83 | 6 |
| | ATOM | 2070 | C | GLY | A | 270 | 32.341 | 32.563 | -22.463 | 1.00 | 32.39 | 6 |
| | ATOM | 2071 | O | GLY | A | 270 | 33.549 | 32.829 | -22.369 | 1.00 | 32.69 | 8 |
| 25 | ATOM | 2072 | N | ASP | A | 271 | 31.552 | 32.562 | -21.390 | 1.00 | 30.56 | 7 |
| | ATOM | 2073 | CA | ASP | A | 271 | 32.088 | 32.888 | -20.075 | 1.00 | 31.93 | 6 |
| | ATOM | 2074 | C | ASP | A | 271 | 32.450 | 31.649 | -19.271 | 1.00 | 31.25 | 6 |
| | ATOM | 2075 | O | ASP | A | 271 | 32.749 | 31.710 | -18.079 | 1.00 | 30.60 | 8 |
| | ATOM | 2076 | CB | ASP | A | 271 | 31.087 | 33.758 | -19.289 | 1.00 | 33.98 | 6 |
| 30 | ATOM | 2077 | CG | ASP | A | 271 | 31.073 | 35.165 | -19.921 | 1.00 | 37.85 | 6 |
| | ATOM | 2078 | OD1 | ASP | A | 271 | 32.103 | 35.682 | -20.401 | 1.00 | 38.52 | 8 |
| | ATOM | 2079 | OD2 | ASP | A | 271 | 29.996 | 35.770 | -19.944 | 1.00 | 39.53 | 8 |
| | ATOM | 2080 | N | ALA | A | 272 | 32.462 | 30.482 | -19.903 | 1.00 | 29.77 | 7 |
| | ATOM | 2081 | CA | ALA | A | 272 | 32.828 | 29.254 | -19.228 | 1.00 | 27.77 | 6 |
| 35 | ATOM | 2082 | C | ALA | A | 272 | 34.256 | 28.826 | -19.557 | 1.00 | 26.45 | 6 |
| | ATOM | 2083 | O | ALA | A | 272 | 34.545 | 28.837 | -20.745 | 1.00 | 26.44 | 8 |
| | ATOM | 2084 | CB | ALA | A | 272 | 31.977 | 28.068 | -19.666 | 1.00 | 27.56 | 6 |
| | ATOM | 2085 | N | ARG | A | 273 | 35.053 | 28.448 | -18.602 | 1.00 | 25.11 | 7 |
| | ATOM | 2086 | CA | ARG | A | 273 | 36.354 | 27.839 | -18.859 | 1.00 | 25.96 | 6 |
| 40 | ATOM | 2087 | C | ARG | A | 273 | 36.194 | 26.346 | -18.606 | 1.00 | 23.79 | 6 |
| | ATOM | 2088 | O | ARG | A | 273 | 36.292 | 25.868 | -17.465 | 1.00 | 25.36 | 8 |
| | ATOM | 2089 | CB | ARG | A | 273 | 37.467 | 28.400 | -17.962 | 1.00 | 27.51 | 6 |
| | ATOM | 2090 | CG | ARG | A | 273 | 38.864 | 27.853 | -18.355 | 1.00 | 27.52 | 6 |
| | ATOM | 2091 | CD | ARG | A | 273 | 39.848 | 28.605 | -17.421 | 1.00 | 28.40 | 6 |
| 45 | ATOM | 2092 | NE | ARG | A | 273 | 41.215 | 28.212 | -17.720 | 0.50 | 26.25 | 7 |
| | ATOM | 2093 | CZ | ARG | A | 273 | 41.850 | 27.144 | -17.306 | 0.50 | 26.10 | 6 |
| | ATOM | 2094 | NH1 | ARG | A | 273 | 41.229 | 26.281 | -16.517 | 0.50 | 28.04 | 7 |
| | ATOM | 2095 | NH2 | ARG | A | 273 | 43.107 | 26.909 | -17.691 | 0.50 | 25.33 | 7 |
| | ATOM | 2096 | N | LEU | A | 274 | 35.918 | 25.587 | -19.693 | 1.00 | 25.09 | 7 |
| 50 | ATOM | 2097 | CA | LEU | A | 274 | 35.608 | 24.173 | -19.545 | 1.00 | 23.10 | 6 |
| | ATOM | 2098 | C | LEU | A | 274 | 36.845 | 23.385 | -19.359 | 1.00 | 23.02 | 6 |
| | ATOM | 2099 | O | LEU | A | 274 | 37.846 | 23.706 | -20.001 | 1.00 | 24.38 | 8 |
| | ATOM | 2100 | CB | LEU | A | 274 | 34.863 | 23.714 | -20.847 | 1.00 | 22.40 | 6 |
| | ATOM | 2101 | CG | LEU | A | 274 | 33.548 | 24.488 | -21.045 | 1.00 | 22.92 | 6 |
| 55 | ATOM | 2102 | CD1 | LEU | A | 274 | 32.953 | 24.119 | -22.368 | 1.00 | 25.59 | 6 |
| | ATOM | 2103 | CD2 | LEU | A | 274 | 32.619 | 24.185 | -19.846 | 1.00 | 24.66 | 6 |
| | ATOM | 2104 | N | ILE | A | 275 | 36.844 | 22.342 | -18.576 | 1.00 | 22.01 | 7 |
| | ATOM | 2105 | CA | ILE | A | 275 | 37.965 | 21.529 | -18.235 | 1.00 | 24.38 | 6 |
| | ATOM | 2106 | C | ILE | A | 275 | 37.640 | 20.072 | -18.439 | 1.00 | 24.31 | 6 |
| 60 | ATOM | 2107 | O | ILE | A | 275 | 36.504 | 19.675 | -18.126 | 1.00 | 23.32 | 8 |
| | ATOM | 2108 | CB | ILE | A | 275 | 38.290 | 21.785 | -16.743 | 1.00 | 27.33 | 6 |
| | ATOM | 2109 | CG1 | ILE | A | 275 | 38.853 | 23.233 | -16.577 | 1.00 | 30.12 | 6 |
| | ATOM | 2110 | CG2 | ILE | A | 275 | 39.295 | 20.826 | -16.161 | 1.00 | 32.15 | 6 |
| | ATOM | 2111 | CD1 | ILE | A | 275 | 38.634 | 23.632 | -15.112 | 1.00 | 33.95 | 6 |
| 65 | ATOM | 2112 | N | ASP | A | 276 | 38.611 | 19.282 | -18.865 | 1.00 | 23.56 | 7 |
| | ATOM | 2113 | CA | ASP | A | 276 | 38.347 | 17.845 | -19.005 | 1.00 | 24.73 | 6 |
| | ATOM | 2114 | C | ASP | A | 276 | 39.702 | 17.125 | -18.966 | 1.00 | 24.26 | 6 |
| | ATOM | 2115 | O | ASP | A | 276 | 40.768 | 17.741 | -19.153 | 1.00 | 24.98 | 8 |
| | ATOM | 2116 | CB | ASP | A | 276 | 37.551 | 17.545 | -20.271 | 1.00 | 24.30 | 6 |
| | ATOM | 2117 | CG | ASP | A | 276 | 36.730 | 16.276 | -20.290 | 1.00 | 26.28 | 6 |
| 70 | ATOM | 2118 | OD1 | ASP | A | 276 | 36.927 | 15.468 | -19.324 | 1.00 | 27.91 | 8 |
| | ATOM | 2119 | OD2 | ASP | A | 276 | 35.946 | 16.119 | -21.251 | 1.00 | 25.73 | 8 |
| | ATOM | 2120 | N | ASN | A | 277 | 39.671 | 15.855 | -18.697 | 1.00 | 22.14 | 7 |
| | ATOM | 2121 | CA | ASN | A | 277 | 40.857 | 15.020 | -18.682 | 1.00 | 25.69 | 6 |
| | ATOM | 2122 | C | ASN | A | 277 | 40.473 | 13.587 | -19.027 | 1.00 | 24.93 | 6 |

-65-

| | | | | | | | | | | |
|----|------|------|-----|-----------|--------|--------|---------|------|-------|----|
| | ATOM | 2123 | O | ASN A 277 | 39.335 | 13.139 | -18.920 | 1.00 | 25.86 | 8 |
| | ATOM | 2124 | CB | ASN A 277 | 41.608 | 15.073 | -17.350 | 1.00 | 28.42 | 6 |
| | ATOM | 2125 | CG | ASN A 277 | 41.077 | 14.298 | -16.164 | 1.00 | 32.43 | 6 |
| 5 | ATOM | 2126 | OD1 | ASN A 277 | 40.715 | 13.140 | -16.247 | 1.00 | 37.45 | 8 |
| | ATOM | 2127 | ND2 | ASN A 277 | 41.023 | 14.889 | -14.994 | 1.00 | 35.65 | 7 |
| | ATOM | 2128 | N | LYS A 278 | 41.517 | 12.825 | -19.428 | 1.00 | 28.31 | 7 |
| | ATOM | 2129 | CA | LYS A 278 | 41.338 | 11.429 | -19.765 | 1.00 | 31.78 | 6 |
| | ATOM | 2130 | C | LYS A 278 | 42.655 | 10.677 | -19.634 | 1.00 | 33.11 | 6 |
| 10 | ATOM | 2131 | O | LYS A 278 | 43.692 | 11.227 | -19.991 | 1.00 | 33.12 | 8 |
| | ATOM | 2132 | CB | LYS A 278 | 40.814 | 11.323 | -21.189 | 1.00 | 32.53 | 6 |
| | ATOM | 2133 | CG | LYS A 278 | 40.748 | 10.008 | -21.905 | 1.00 | 35.09 | 6 |
| | ATOM | 2134 | CD | LYS A 278 | 39.814 | 10.144 | -23.124 | 1.00 | 38.06 | 6 |
| | ATOM | 2135 | CE | LYS A 278 | 39.115 | 8.808 | -23.384 | 1.00 | 39.45 | 6 |
| 15 | ATOM | 2136 | NZ | LYS A 278 | 37.984 | 9.018 | -24.354 | 1.00 | 40.81 | 7 |
| | ATOM | 2137 | N | MET A 279 | 42.594 | 9.455 | -19.139 | 1.00 | 35.39 | 7 |
| | ATOM | 2138 | CA | MET A 279 | 43.799 | 8.636 | -19.046 | 1.00 | 39.07 | 6 |
| | ATOM | 2139 | C | MET A 279 | 43.777 | 7.645 | -20.201 | 1.00 | 40.75 | 6 |
| | ATOM | 2140 | O | MET A 279 | 42.688 | 7.224 | -20.590 | 1.00 | 39.38 | 8 |
| 20 | ATOM | 2141 | CB | MET A 279 | 43.895 | 7.997 | -17.641 | 1.00 | 42.09 | 6 |
| | ATOM | 2142 | CG | MET A 279 | 44.366 | 9.076 | -16.657 | 1.00 | 45.36 | 6 |
| | ATOM | 2143 | SD | MET A 279 | 44.591 | 8.656 | -14.926 | 1.00 | 51.28 | 16 |
| | ATOM | 2144 | CE | MET A 279 | 42.948 | 8.136 | -14.428 | 1.00 | 49.74 | 6 |
| | ATOM | 2145 | N | VAL A 280 | 44.953 | 7.391 | -20.786 | 1.00 | 41.33 | 7 |
| 25 | ATOM | 2146 | CA | VAL A 280 | 44.994 | 6.466 | -21.917 | 1.00 | 44.04 | 6 |
| | ATOM | 2147 | C | VAL A 280 | 46.138 | 5.483 | -21.692 | 1.00 | 45.91 | 6 |
| | ATOM | 2148 | O | VAL A 280 | 47.232 | 5.881 | -21.274 | 1.00 | 44.69 | 8 |
| | ATOM | 2149 | CB | VAL A 280 | 45.126 | 7.195 | -23.265 | 1.00 | 43.07 | 6 |
| | ATOM | 2150 | CG1 | VAL A 280 | 46.430 | 7.978 | -23.326 | 1.00 | 43.41 | 6 |
| 30 | ATOM | 2151 | CG2 | VAL A 280 | 45.060 | 6.239 | -24.439 | 1.00 | 43.94 | 6 |
| | ATOM | 2152 | N | GLU A 281 | 45.787 | 4.211 | -21.867 | 1.00 | 51.13 | 7 |
| | ATOM | 2153 | CA | GLU A 281 | 46.797 | 3.151 | -21.712 | 1.00 | 54.78 | 6 |
| | ATOM | 2154 | C | GLU A 281 | 47.658 | 3.176 | -22.971 | 1.00 | 55.75 | 6 |
| | ATOM | 2155 | O | GLU A 281 | 47.155 | 3.235 | -24.094 | 1.00 | 55.40 | 8 |
| 35 | ATOM | 2156 | CB | GLU A 281 | 46.186 | 1.784 | -21.469 | 1.00 | 56.82 | 6 |
| | ATOM | 2157 | CG | GLU A 281 | 45.244 | 1.658 | -20.296 | 1.00 | 59.30 | 6 |
| | ATOM | 2158 | CD | GLU A 281 | 45.898 | 1.424 | -18.957 | 1.00 | 61.75 | 6 |
| | ATOM | 2159 | OE1 | GLU A 281 | 47.135 | 1.218 | -18.919 | 1.00 | 62.80 | 8 |
| | ATOM | 2160 | OE2 | GLU A 281 | 45.187 | 1.411 | -17.923 | 1.00 | 62.74 | 8 |
| 40 | ATOM | 2161 | N | LEU A 282 | 48.958 | 3.235 | -22.781 | 1.00 | 57.94 | 7 |
| | ATOM | 2162 | CA | LEU A 282 | 49.944 | 3.334 | -23.844 | 1.00 | 60.20 | 6 |
| | ATOM | 2163 | C | LEU A 282 | 50.394 | 1.966 | -24.343 | 1.00 | 62.75 | 6 |
| | ATOM | 2164 | O | LEU A 282 | 50.792 | 1.813 | -25.501 | 1.00 | 63.61 | 8 |
| | ATOM | 2165 | CB | LEU A 282 | 51.132 | 4.160 | -23.353 | 1.00 | 60.14 | 6 |
| 45 | ATOM | 2166 | CG | LEU A 282 | 51.250 | 5.643 | -23.655 | 1.00 | 59.64 | 6 |
| | ATOM | 2167 | CD1 | LEU A 282 | 49.954 | 6.281 | -24.103 | 1.00 | 59.72 | 6 |
| | ATOM | 2168 | CD2 | LEU A 282 | 51.880 | 6.386 | -22.494 | 1.00 | 58.92 | 6 |
| | ATOM | 2169 | N | ALA A 283 | 50.285 | 0.961 | -23.484 | 1.00 | 64.72 | 7 |
| | ATOM | 2170 | CA | ALA A 283 | 50.637 | -0.410 | -23.818 | 1.00 | 66.41 | 6 |
| 50 | ATOM | 2171 | C | ALA A 283 | 49.397 | -1.291 | -23.933 | 1.00 | 67.10 | 6 |
| | ATOM | 2172 | O | ALA A 283 | 48.394 | -0.879 | -24.563 | 1.00 | 68.25 | 8 |
| | ATOM | 2173 | CB | ALA A 283 | 51.563 | -1.007 | -22.764 | 1.00 | 66.62 | 6 |

55 Monomer B

| | | | Atom type | | | | X | Y | Z | Occ. | B | Atomic No. |
|----|------|------|--------------|-----|---|---|--------|---------|--------|------|-------|---------------|
| 60 | ATOM | 2174 | N | MET | B | 1 | 58.003 | -23.593 | 11.263 | 1.00 | 36.48 | 7 |
| | ATOM | 2175 | CA | MET | B | 1 | 58.132 | -22.126 | 11.083 | 1.00 | 33.40 | 6 |
| | ATOM | 2176 | C | MET | B | 1 | 58.194 | -21.749 | 9.627 | 1.00 | 33.88 | 6 |
| | ATOM | 2177 | O | MET | B | 1 | 59.003 | -22.271 | 8.843 | 1.00 | 34.96 | 8 |
| 65 | ATOM | 2178 | CB | MET | B | 1 | 59.383 | -21.686 | 11.860 | 1.00 | 32.85 | 6 |
| | ATOM | 2179 | CG | MET | B | 1 | 59.602 | -20.178 | 11.711 | 1.00 | 32.05 | 6 |
| | ATOM | 2180 | SD | MET | B | 1 | 61.001 | -19.706 | 12.738 | 1.00 | 32.48 | 16 |
| | ATOM | 2181 | CE | MET | B | 1 | 62.316 | -19.795 | 11.507 | 1.00 | 33.02 | 6 |
| 70 | ATOM | 2182 | N | LEU | B | 2 | 57.366 | -20.850 | 9.145 | 1.00 | 30.67 | 7 |
| | ATOM | 2183 | CA | LEU | B | 2 | 57.332 | -20.400 | 7.790 | 1.00 | 31.35 | 6 |
| | ATOM | 2184 | C | LEU | B | 2 | 58.315 | -19.246 | 7.576 | 1.00 | 32.39 | 6 |
| | ATOM | 2185 | O | LEU | B | 2 | 58.367 | -18.394 | 8.491 | 1.00 | 31.76 | 8 |
| | ATOM | 2186 | CB | LEU | B | 2 | 55.926 | -19.896 | 7.473 | 1.00 | 35.48 | 6 |
| | ATOM | 2187 | CG | LEU | B | 2 | 54.773 | -20.875 | 7.670 | 1.00 | 38.24 | 6 |
| | ATOM | 2188 | CD1 | LEU | B | 2 | 53.410 | -20.187 | 7.668 | 1.00 | 37.95 | 6 |

-66-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| | ATOM | 2189 | CD2 | LEU | B | 2 | 54.803 | -21.930 | 6.560 | 1.00 | 38.99 | 6 |
| | ATOM | 2190 | N | ILE | B | 3 | 58.980 | -19.217 | 6.439 | 1.00 | 28.48 | 7 |
| | ATOM | 2191 | CA | ILE | B | 3 | 59.916 | -18.162 | 6.099 | 1.00 | 29.00 | 6 |
| 5 | ATOM | 2192 | C | ILE | B | 3 | 59.442 | -17.553 | 4.806 | 1.00 | 30.65 | 6 |
| | ATOM | 2193 | O | ILE | B | 3 | 59.350 | -18.257 | 3.778 | 1.00 | 31.80 | 8 |
| | ATOM | 2194 | CB | ILE | B | 3 | 61.380 | -18.634 | 5.938 | 1.00 | 31.56 | 6 |
| | ATOM | 2195 | CG1 | ILE | B | 3 | 61.859 | -19.222 | 7.261 | 1.00 | 31.29 | 6 |
| | ATOM | 2196 | CG2 | ILE | B | 3 | 62.257 | -17.481 | 5.477 | 1.00 | 32.77 | 6 |
| 10 | ATOM | 2197 | CD1 | ILE | B | 3 | 63.283 | -19.769 | 7.266 | 1.00 | 37.37 | 6 |
| | ATOM | 2198 | N | ILE | B | 4 | 58.918 | -16.333 | 4.826 | 1.00 | 24.55 | 7 |
| | ATOM | 2199 | CA | ILE | B | 4 | 58.284 | -15.663 | 3.748 | 1.00 | 26.13 | 6 |
| | ATOM | 2200 | C | ILE | B | 4 | 59.159 | -14.534 | 3.279 | 1.00 | 28.00 | 6 |
| | ATOM | 2201 | O | ILE | B | 4 | 59.649 | -13.738 | 4.079 | 1.00 | 28.39 | 8 |
| 15 | ATOM | 2202 | CB | ILE | B | 4 | 56.926 | -15.034 | 4.179 | 1.00 | 26.38 | 6 |
| | ATOM | 2203 | CG1 | ILE | B | 4 | 56.042 | -16.103 | 4.827 | 1.00 | 30.33 | 6 |
| | ATOM | 2204 | CG2 | ILE | B | 4 | 56.248 | -14.318 | 3.013 | 1.00 | 28.07 | 6 |
| | ATOM | 2205 | CD1 | ILE | B | 4 | 55.611 | -17.272 | 3.955 | 1.00 | 30.56 | 6 |
| | ATOM | 2206 | N | GLU | B | 5 | 59.374 | -14.485 | 1.987 | 1.00 | 29.37 | 7 |
| 20 | ATOM | 2207 | CA | GLU | B | 5 | 60.209 | -13.449 | 1.380 | 1.00 | 31.10 | 6 |
| | ATOM | 2208 | C | GLU | B | 5 | 59.387 | -12.614 | 0.487 | 1.00 | 30.29 | 6 |
| | ATOM | 2209 | O | GLU | B | 5 | 59.982 | -11.574 | 0.059 | 1.00 | 32.17 | 8 |
| | ATOM | 2210 | CB | GLU | B | 5 | 61.292 | -14.267 | 0.655 | 1.00 | 35.81 | 6 |
| | ATOM | 2211 | CG | GLU | B | 5 | 62.267 | -15.017 | 1.547 | 1.00 | 40.51 | 6 |
| 25 | ATOM | 2212 | CD | GLU | B | 5 | 63.167 | -15.907 | 0.709 | 1.00 | 45.93 | 6 |
| | ATOM | 2213 | OE1 | GLU | B | 5 | 63.562 | -16.994 | 1.195 | 1.00 | 48.88 | 8 |
| | ATOM | 2214 | OE2 | GLU | B | 5 | 63.451 | -15.521 | -0.447 | 1.00 | 46.38 | 8 |
| | ATOM | 2215 | N | THR | B | 6 | 58.142 | -12.721 | 0.076 | 1.00 | 26.13 | 7 |
| | ATOM | 2216 | CA | THR | B | 6 | 57.578 | -11.758 | -0.836 | 1.00 | 27.91 | 6 |
| 30 | ATOM | 2217 | C | THR | B | 6 | 56.298 | -11.128 | -0.207 | 1.00 | 24.93 | 6 |
| | ATOM | 2218 | O | THR | B | 6 | 55.656 | -11.788 | 0.619 | 1.00 | 27.98 | 8 |
| | ATOM | 2219 | CB | THR | B | 6 | 57.229 | -12.351 | -2.205 | 1.00 | 31.04 | 6 |
| | ATOM | 2220 | OG1 | THR | B | 6 | 56.159 | -13.300 | -2.052 | 1.00 | 30.86 | 8 |
| | ATOM | 2221 | CG2 | THR | B | 6 | 58.425 | -13.076 | -2.851 | 1.00 | 31.94 | 6 |
| 35 | ATOM | 2222 | N | LEU | B | 7 | 55.927 | -10.037 | -0.790 | 1.00 | 27.39 | 7 |
| | ATOM | 2223 | CA | LEU | B | 7 | 54.715 | -9.308 | -0.367 | 1.00 | 28.55 | 6 |
| | ATOM | 2224 | C | LEU | B | 7 | 53.455 | -10.153 | -0.636 | 1.00 | 27.46 | 6 |
| | ATOM | 2225 | O | LEU | B | 7 | 52.669 | -10.343 | 0.308 | 1.00 | 26.58 | 8 |
| | ATOM | 2226 | CB | LEU | B | 7 | 54.583 | -7.921 | -0.986 | 1.00 | 29.88 | 6 |
| 40 | ATOM | 2227 | CG | LEU | B | 7 | 55.750 | -6.939 | -0.729 | 1.00 | 31.25 | 6 |
| | ATOM | 2228 | CD1 | LEU | B | 7 | 55.361 | -5.499 | -1.043 | 1.00 | 31.80 | 6 |
| | ATOM | 2229 | CD2 | LEU | B | 7 | 56.271 | -7.052 | 0.703 | 1.00 | 30.25 | 6 |
| | ATOM | 2230 | N | PRO | B | 8 | 53.288 | -10.697 | -1.811 | 1.00 | 28.20 | 7 |
| | ATOM | 2231 | CA | PRO | B | 8 | 52.092 | -11.501 | -2.092 | 1.00 | 28.01 | 6 |
| 45 | ATOM | 2232 | C | PRO | B | 8 | 51.973 | -12.671 | -1.172 | 1.00 | 27.27 | 6 |
| | ATOM | 2233 | O | PRO | B | 8 | 50.869 | -12.943 | -0.641 | 1.00 | 26.76 | 8 |
| | ATOM | 2234 | CB | PRO | B | 8 | 52.264 | -11.941 | -3.550 | 1.00 | 30.16 | 6 |
| | ATOM | 2235 | CG | PRO | B | 8 | 53.126 | -10.877 | -4.147 | 1.00 | 30.87 | 6 |
| | ATOM | 2236 | CD | PRO | B | 8 | 54.088 | -10.500 | -3.047 | 1.00 | 28.88 | 6 |
| 50 | ATOM | 2237 | N | LEU | B | 9 | 53.045 | -13.427 | -0.954 | 1.00 | 25.43 | 7 |
| | ATOM | 2238 | CA | LEU | B | 9 | 53.054 | -14.599 | -0.088 | 1.00 | 25.93 | 6 |
| | ATOM | 2239 | C | LEU | B | 9 | 52.839 | -14.206 | 1.363 | 1.00 | 27.59 | 6 |
| | ATOM | 2240 | O | LEU | B | 9 | 52.069 | -14.843 | 2.081 | 1.00 | 25.94 | 8 |
| | ATOM | 2241 | CB | LEU | B | 9 | 54.355 | -15.416 | -0.317 | 1.00 | 27.71 | 6 |
| 55 | ATOM | 2242 | CG | LEU | B | 9 | 54.311 | -16.200 | -1.656 | 1.00 | 31.97 | 6 |
| | ATOM | 2243 | CD1 | LEU | B | 9 | 55.671 | -16.790 | -1.961 | 1.00 | 30.14 | 6 |
| | ATOM | 2244 | CD2 | LEU | B | 9 | 53.236 | -17.279 | -1.607 | 1.00 | 32.64 | 6 |
| | ATOM | 2245 | N | LEU | B | 10 | 53.323 | -13.028 | 1.819 | 1.00 | 25.26 | 7 |
| | ATOM | 2246 | CA | LEU | B | 10 | 53.068 | -12.583 | 3.182 | 1.00 | 23.45 | 6 |
| 60 | ATOM | 2247 | C | LEU | B | 10 | 51.581 | -12.234 | 3.362 | 1.00 | 22.04 | 6 |
| | ATOM | 2248 | O | LEU | B | 10 | 50.941 | -12.683 | 4.336 | 1.00 | 22.46 | 8 |
| | ATOM | 2249 | CB | LEU | B | 10 | 53.963 | -11.368 | 3.535 | 1.00 | 25.32 | 6 |
| | ATOM | 2250 | CG | LEU | B | 10 | 53.618 | -10.738 | 4.917 | 1.00 | 23.24 | 6 |
| | ATOM | 2251 | CD1 | LEU | B | 10 | 53.904 | -11.665 | 6.068 | 1.00 | 21.41 | 6 |
| 65 | ATOM | 2252 | CD2 | LEU | B | 10 | 54.376 | -9.417 | 5.105 | 1.00 | 22.97 | 6 |
| | ATOM | 2253 | N | ARG | B | 11 | 50.992 | -11.537 | 2.407 | 1.00 | 23.80 | 7 |
| | ATOM | 2254 | CA | ARG | B | 11 | 49.591 | -11.130 | 2.459 | 1.00 | 26.88 | 6 |
| | ATOM | 2255 | C | ARG | B | 11 | 48.681 | -12.350 | 2.583 | 1.00 | 26.18 | 6 |
| | ATOM | 2256 | O | ARG | B | 11 | 47.707 | -12.322 | 3.328 | 1.00 | 23.87 | 8 |
| 70 | ATOM | 2257 | CB | ARG | B | 11 | 49.208 | -10.303 | 1.232 | 1.00 | 26.73 | 6 |
| | ATOM | 2258 | CG | ARG | B | 11 | 49.968 | -8.984 | 1.209 | 1.00 | 29.98 | 6 |
| | ATOM | 2259 | CD | ARG | B | 11 | 49.306 | -7.986 | 0.278 | 1.00 | 35.78 | 6 |
| | ATOM | 2260 | NE | ARG | B | 11 | 49.673 | -6.602 | 0.492 | 1.00 | 38.73 | 7 |
| | ATOM | 2261 | CZ | ARG | B | 11 | 50.447 | -5.830 | -0.254 | 1.00 | 39.79 | 6 |
| | ATOM | 2262 | NH1 | ARG | B | 11 | 51.031 | -6.255 | -1.376 | 1.00 | 41.64 | 7 |

-67-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| | ATOM | 2263 | NH2 | ARG | B | 11 | 50.651 | -4.546 | 0.070 | 1.00 | 40.26 | 7 |
| | ATOM | 2264 | N | GLN | B | 12 | 48.992 | -13.409 | 1.864 | 1.00 | 24.75 | 7 |
| | ATOM | 2265 | CA | GLN | B | 12 | 48.289 | -14.712 | 1.885 | 1.00 | 23.93 | 6 |
| 5 | ATOM | 2266 | C | GLN | B | 12 | 48.282 | -15.281 | 3.285 | 1.00 | 23.24 | 6 |
| | ATOM | 2267 | O | GLN | B | 12 | 47.231 | -15.711 | 3.804 | 1.00 | 23.11 | 8 |
| | ATOM | 2268 | CB | GLN | B | 12 | 48.919 | -15.669 | 0.879 | 1.00 | 25.20 | 6 |
| | ATOM | 2269 | CG | GLN | B | 12 | 48.494 | -17.114 | 0.983 | 1.00 | 31.10 | 6 |
| | ATOM | 2270 | CD | GLN | B | 12 | 48.983 | -18.004 | -0.160 | 1.00 | 33.85 | 6 |
| 10 | ATOM | 2271 | OE1 | GLN | B | 12 | 50.160 | -18.359 | -0.226 | 1.00 | 34.46 | 8 |
| | ATOM | 2272 | NE2 | GLN | B | 12 | 48.024 | -18.373 | -1.035 | 1.00 | 37.05 | 7 |
| | ATOM | 2273 | N | GLN | B | 13 | 49.406 | -15.241 | 4.018 | 1.00 | 20.76 | 7 |
| | ATOM | 2274 | CA | GLN | B | 13 | 49.531 | -15.725 | 5.367 | 1.00 | 21.58 | 6 |
| | ATOM | 2275 | C | GLN | B | 13 | 48.755 | -14.802 | 6.342 | 1.00 | 19.88 | 6 |
| 15 | ATOM | 2276 | O | GLN | B | 13 | 48.070 | -15.312 | 7.250 | 1.00 | 20.12 | 8 |
| | ATOM | 2277 | CB | GLN | B | 13 | 51.005 | -15.852 | 5.844 | 1.00 | 22.55 | 6 |
| | ATOM | 2278 | CG | GLN | B | 13 | 51.779 | -16.951 | 5.087 | 1.00 | 25.94 | 6 |
| | ATOM | 2279 | CD | GLN | B | 13 | 51.107 | -18.297 | 5.150 | 1.00 | 27.86 | 6 |
| | ATOM | 2280 | OE1 | GLN | B | 13 | 50.677 | -18.693 | 6.225 | 1.00 | 28.91 | 8 |
| 20 | ATOM | 2281 | NE2 | GLN | B | 13 | 50.985 | -18.937 | 3.993 | 1.00 | 32.63 | 7 |
| | ATOM | 2282 | N | ILE | B | 14 | 48.738 | -13.510 | 6.042 | 1.00 | 21.05 | 7 |
| | ATOM | 2283 | CA | ILE | B | 14 | 48.035 | -12.575 | 6.947 | 1.00 | 20.18 | 6 |
| | ATOM | 2284 | C | ILE | B | 14 | 46.501 | -12.822 | 6.819 | 1.00 | 21.51 | 6 |
| | ATOM | 2285 | O | ILE | B | 14 | 45.800 | -12.838 | 7.850 | 1.00 | 21.76 | 8 |
| 25 | ATOM | 2286 | CB | ILE | B | 14 | 48.438 | -11.133 | 6.718 | 1.00 | 21.52 | 6 |
| | ATOM | 2287 | CG1 | ILE | B | 14 | 49.931 | -10.873 | 7.014 | 1.00 | 21.53 | 6 |
| | ATOM | 2288 | CG2 | ILE | B | 14 | 47.609 | -10.137 | 7.572 | 1.00 | 20.30 | 6 |
| | ATOM | 2289 | CD1 | ILE | B | 14 | 50.448 | -11.493 | 8.287 | 1.00 | 20.36 | 6 |
| | ATOM | 2290 | N | ARG | B | 15 | 46.060 | -13.042 | 5.580 | 1.00 | 21.97 | 7 |
| 30 | ATOM | 2291 | CA | ARG | B | 15 | 44.640 | -13.407 | 5.403 | 1.00 | 21.03 | 6 |
| | ATOM | 2292 | C | ARG | B | 15 | 44.328 | -14.704 | 6.120 | 1.00 | 20.84 | 6 |
| | ATOM | 2293 | O | ARG | B | 15 | 43.231 | -14.819 | 6.693 | 1.00 | 21.21 | 8 |
| | ATOM | 2294 | CB | ARG | B | 15 | 44.362 | -13.468 | 3.903 | 1.00 | 23.95 | 6 |
| | ATOM | 2295 | CG | ARG | B | 15 | 44.439 | -12.110 | 3.182 | 1.00 | 28.33 | 6 |
| 35 | ATOM | 2296 | CD | ARG | B | 15 | 43.633 | -12.304 | 1.885 | 1.00 | 35.29 | 6 |
| | ATOM | 2297 | NE | ARG | B | 15 | 44.463 | -13.095 | 0.938 | 1.00 | 39.61 | 7 |
| | ATOM | 2298 | CZ | ARG | B | 15 | 45.378 | -12.352 | 0.272 | 1.00 | 43.48 | 6 |
| | ATOM | 2299 | NH1 | ARG | B | 15 | 45.533 | -11.036 | 0.426 | 1.00 | 44.40 | 7 |
| | ATOM | 2300 | NH2 | ARG | B | 15 | 46.158 | -12.973 | -0.594 | 1.00 | 43.72 | 7 |
| 40 | ATOM | 2301 | N | ARG | B | 16 | 45.189 | -15.724 | 6.069 | 1.00 | 18.66 | 7 |
| | ATOM | 2302 | CA | ARG | B | 16 | 44.923 | -16.986 | 6.717 | 1.00 | 19.99 | 6 |
| | ATOM | 2303 | C | ARG | B | 16 | 44.816 | -16.743 | 8.234 | 1.00 | 20.42 | 6 |
| | ATOM | 2304 | O | ARG | B | 16 | 43.855 | -17.229 | 8.824 | 1.00 | 19.70 | 8 |
| | ATOM | 2305 | CB | ARG | B | 16 | 45.959 | -18.073 | 6.435 | 1.00 | 22.24 | 6 |
| 45 | ATOM | 2306 | CG | ARG | B | 16 | 45.869 | -19.264 | 7.352 | 1.00 | 23.29 | 6 |
| | ATOM | 2307 | CD | ARG | B | 16 | 46.986 | -20.277 | 7.132 | 1.00 | 25.24 | 6 |
| | ATOM | 2308 | NE | ARG | B | 16 | 48.309 | -19.702 | 7.470 | 1.00 | 27.88 | 7 |
| | ATOM | 2309 | CZ | ARG | B | 16 | 48.797 | -19.716 | 8.706 | 1.00 | 28.92 | 6 |
| | ATOM | 2310 | NH1 | ARG | B | 16 | 50.016 | -19.215 | 8.961 | 1.00 | 28.52 | 7 |
| 50 | ATOM | 2311 | NH2 | ARG | B | 16 | 48.126 | -20.327 | 9.679 | 1.00 | 24.92 | 7 |
| | ATOM | 2312 | N | LEU | B | 17 | 45.716 | -15.933 | 8.815 | 1.00 | 19.27 | 7 |
| | ATOM | 2313 | CA | LEU | B | 17 | 45.626 | -15.699 | 10.270 | 1.00 | 20.77 | 6 |
| | ATOM | 2314 | C | LEU | B | 17 | 44.352 | -14.990 | 10.702 | 1.00 | 20.30 | 6 |
| | ATOM | 2315 | O | LEU | B | 17 | 43.778 | -15.286 | 11.759 | 1.00 | 19.03 | 8 |
| 55 | ATOM | 2316 | CB | LEU | B | 17 | 46.900 | -14.923 | 10.697 | 1.00 | 22.28 | 6 |
| | ATOM | 2317 | CG | LEU | B | 17 | 48.154 | -15.834 | 10.589 | 1.00 | 20.91 | 6 |
| | ATOM | 2318 | CD1 | LEU | B | 17 | 49.346 | -14.854 | 10.747 | 1.00 | 23.26 | 6 |
| | ATOM | 2319 | CD2 | LEU | B | 17 | 48.210 | -16.976 | 11.546 | 1.00 | 23.26 | 6 |
| | ATOM | 2320 | N | ARG | B | 18 | 43.880 | -14.084 | 9.852 | 1.00 | 20.08 | 7 |
| 60 | ATOM | 2321 | CA | ARG | B | 18 | 42.616 | -13.394 | 10.085 | 1.00 | 20.19 | 6 |
| | ATOM | 2322 | C | ARG | B | 18 | 41.443 | -14.367 | 10.053 | 1.00 | 20.24 | 6 |
| | ATOM | 2323 | O | ARG | B | 18 | 40.595 | -14.419 | 10.938 | 1.00 | 19.77 | 8 |
| | ATOM | 2324 | CB | ARG | B | 18 | 42.410 | -12.287 | 9.049 | 1.00 | 19.52 | 6 |
| | ATOM | 2325 | CG | ARG | B | 18 | 41.388 | -11.239 | 9.456 | 1.00 | 25.28 | 6 |
| 65 | ATOM | 2326 | CD | ARG | B | 18 | 40.953 | -10.402 | 8.264 | 1.00 | 30.78 | 6 |
| | ATOM | 2327 | NE | ARG | B | 18 | 42.033 | -9.556 | 7.766 | 1.00 | 37.79 | 7 |
| | ATOM | 2328 | CZ | ARG | B | 18 | 42.285 | -9.348 | 6.478 | 1.00 | 41.34 | 6 |
| | ATOM | 2329 | NH1 | ARG | B | 18 | 41.532 | -9.927 | 5.553 | 1.00 | 41.84 | 7 |
| | ATOM | 2330 | NH2 | ARG | B | 18 | 43.290 | -8.562 | 6.119 | 1.00 | 42.14 | 7 |
| 70 | ATOM | 2331 | N | MET | B | 19 | 41.447 | -15.266 | 9.053 | 1.00 | 19.56 | 7 |
| | ATOM | 2332 | CA | MET | B | 19 | 40.384 | -16.272 | 8.983 | 1.00 | 21.07 | 6 |
| | ATOM | 2333 | C | MET | B | 19 | 40.376 | -17.192 | 10.199 | 1.00 | 19.93 | 6 |
| | ATOM | 2334 | O | MET | B | 19 | 39.291 | -17.611 | 10.629 | 1.00 | 18.95 | 8 |
| | ATOM | 2335 | CB | MET | B | 19 | 40.507 | -17.047 | 7.683 | 1.00 | 21.11 | 6 |
| | ATOM | 2336 | CG | MET | B | 19 | 39.650 | -18.307 | 7.449 | 1.00 | 22.70 | 6 |

-68-

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|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|----|
| | ATOM | 2337 | SD | MET | B | 19 | 40.253 | -19.824 | 8.206 | 1.00 | 21.29 | 16 |
| | ATOM | 2338 | CE | MET | B | 19 | 41.816 | -20.143 | 7.368 | 1.00 | 22.90 | 6 |
| | ATOM | 2339 | N | GLU | B | 20 | 41.516 | -17.512 | 10.731 | 1.00 | 18.16 | 7 |
| 5 | ATOM | 2340 | CA | GLU | B | 20 | 41.687 | -18.429 | 11.858 | 1.00 | 20.12 | 6 |
| | ATOM | 2341 | C | GLU | B | 20 | 41.280 | -17.732 | 13.182 | 1.00 | 20.85 | 6 |
| | ATOM | 2342 | O | GLU | B | 20 | 41.156 | -18.387 | 14.243 | 1.00 | 24.28 | 8 |
| | ATOM | 2343 | CB | GLU | B | 20 | 43.113 | -18.960 | 11.945 | 1.00 | 18.82 | 6 |
| | ATOM | 2344 | CG | GLU | B | 20 | 43.467 | -19.977 | 10.846 | 1.00 | 21.83 | 6 |
| 10 | ATOM | 2345 | CD | GLU | B | 20 | 44.911 | -20.433 | 10.890 | 1.00 | 26.79 | 6 |
| | ATOM | 2346 | OE1 | GLU | B | 20 | 45.611 | -20.063 | 11.869 | 1.00 | 28.93 | 8 |
| | ATOM | 2347 | OE2 | GLU | B | 20 | 45.312 | -21.210 | 9.985 | 1.00 | 26.44 | 8 |
| | ATOM | 2348 | N | GLY | B | 21 | 41.236 | -16.424 | 13.172 | 1.00 | 21.16 | 7 |
| | ATOM | 2349 | CA | GLY | B | 21 | 40.877 | -15.568 | 14.299 | 1.00 | 20.08 | 6 |
| 15 | ATOM | 2350 | C | GLY | B | 21 | 42.055 | -15.540 | 15.311 | 1.00 | 21.45 | 6 |
| | ATOM | 2351 | O | GLY | B | 21 | 41.856 | -15.580 | 16.546 | 1.00 | 20.95 | 8 |
| | ATOM | 2352 | N | LYS | B | 22 | 43.279 | -15.515 | 14.815 | 1.00 | 17.96 | 7 |
| | ATOM | 2353 | CA | LYS | B | 22 | 44.458 | -15.503 | 15.668 | 1.00 | 21.37 | 6 |
| | ATOM | 2354 | C | LYS | B | 22 | 44.924 | -14.091 | 15.953 | 1.00 | 23.78 | 6 |
| 20 | ATOM | 2355 | O | LYS | B | 22 | 44.942 | -13.267 | 15.041 | 1.00 | 24.76 | 8 |
| | ATOM | 2356 | CB | LYS | B | 22 | 45.638 | -16.191 | 14.984 | 1.00 | 22.71 | 6 |
| | ATOM | 2357 | CG | LYS | B | 22 | 45.420 | -17.662 | 14.646 | 1.00 | 25.81 | 6 |
| | ATOM | 2358 | CD | LYS | B | 22 | 45.337 | -18.553 | 15.836 | 1.00 | 28.29 | 6 |
| | ATOM | 2359 | CE | LYS | B | 22 | 44.963 | -19.997 | 15.550 | 1.00 | 33.33 | 6 |
| 25 | ATOM | 2360 | NZ | LYS | B | 22 | 45.832 | -20.715 | 14.575 | 1.00 | 29.69 | 7 |
| | ATOM | 2361 | N | ARG | B | 23 | 45.285 | -13.775 | 17.175 | 1.00 | 19.63 | 7 |
| | ATOM | 2362 | CA | ARG | B | 23 | 45.917 | -12.467 | 17.446 | 1.00 | 22.19 | 6 |
| | ATOM | 2363 | C | ARG | B | 23 | 47.415 | -12.521 | 17.203 | 1.00 | 20.99 | 6 |
| | ATOM | 2364 | O | ARG | B | 23 | 48.014 | -13.529 | 17.533 | 1.00 | 22.27 | 8 |
| 30 | ATOM | 2365 | CB | ARG | B | 23 | 45.620 | -12.042 | 18.877 | 1.00 | 23.98 | 6 |
| | ATOM | 2366 | CG | ARG | B | 23 | 44.149 | -11.748 | 19.161 | 1.00 | 33.05 | 6 |
| | ATOM | 2367 | CD | ARG | B | 23 | 43.965 | -11.207 | 20.600 | 1.00 | 35.95 | 6 |
| | ATOM | 2368 | NE | ARG | B | 23 | 44.774 | -11.865 | 21.560 | 1.00 | 39.00 | 7 |
| | ATOM | 2369 | CZ | ARG | B | 23 | 45.045 | -12.903 | 22.319 | 1.00 | 38.30 | 6 |
| 35 | ATOM | 2370 | NH1 | ARG | B | 23 | 44.343 | -14.060 | 22.457 | 1.00 | 34.37 | 7 |
| | ATOM | 2371 | NH2 | ARG | B | 23 | 46.204 | -12.653 | 22.881 | 1.00 | 33.10 | 7 |
| | ATOM | 2372 | N | VAL | B | 24 | 47.873 | -11.534 | 16.444 | 1.00 | 19.44 | 7 |
| | ATOM | 2373 | CA | VAL | B | 24 | 49.260 | -11.534 | 15.984 | 1.00 | 19.87 | 6 |
| | ATOM | 2374 | C | VAL | B | 24 | 50.133 | -10.493 | 16.615 | 1.00 | 20.77 | 6 |
| 40 | ATOM | 2375 | O | VAL | B | 24 | 49.724 | -9.356 | 16.770 | 1.00 | 20.17 | 8 |
| | ATOM | 2376 | CB | VAL | B | 24 | 49.220 | -11.301 | 14.473 | 1.00 | 20.82 | 6 |
| | ATOM | 2377 | CG1 | VAL | B | 24 | 50.587 | -11.071 | 13.856 | 1.00 | 21.58 | 6 |
| | ATOM | 2378 | CG2 | VAL | B | 24 | 48.493 | -12.516 | 13.838 | 1.00 | 22.44 | 6 |
| | ATOM | 2379 | N | ALA | B | 25 | 51.327 | -10.950 | 17.072 | 1.00 | 18.32 | 7 |
| 45 | ATOM | 2380 | CA | ALA | B | 25 | 52.294 | -9.989 | 17.591 | 1.00 | 18.65 | 6 |
| | ATOM | 2381 | C | ALA | B | 25 | 53.431 | -9.885 | 16.600 | 1.00 | 22.09 | 6 |
| | ATOM | 2382 | O | ALA | B | 25 | 53.908 | -10.915 | 16.053 | 1.00 | 26.60 | 8 |
| | ATOM | 2383 | CB | ALA | B | 25 | 52.871 | -10.371 | 18.953 | 1.00 | 20.06 | 6 |
| | ATOM | 2384 | N | LEU | B | 26 | 53.922 | -8.705 | 16.329 | 1.00 | 18.28 | 7 |
| 50 | ATOM | 2385 | CA | LEU | B | 26 | 54.997 | -8.468 | 15.410 | 1.00 | 16.76 | 6 |
| | ATOM | 2386 | C | LEU | B | 26 | 56.273 | -8.010 | 16.156 | 1.00 | 20.96 | 6 |
| | ATOM | 2387 | O | LEU | B | 26 | 56.139 | -7.157 | 17.020 | 1.00 | 21.27 | 8 |
| | ATOM | 2388 | CB | LEU | B | 26 | 54.673 | -7.425 | 14.340 | 1.00 | 19.09 | 6 |
| | ATOM | 2389 | CG | LEU | B | 26 | 55.816 | -6.890 | 13.487 | 1.00 | 19.40 | 6 |
| 55 | ATOM | 2390 | CD1 | LEU | B | 26 | 56.464 | -7.969 | 12.603 | 1.00 | 21.45 | 6 |
| | ATOM | 2391 | CD2 | LEU | B | 26 | 55.320 | -5.738 | 12.604 | 1.00 | 22.40 | 6 |
| | ATOM | 2392 | N | VAL | B | 27 | 57.396 | -8.642 | 15.874 | 1.00 | 20.49 | 7 |
| | ATOM | 2393 | CA | VAL | B | 27 | 58.684 | -8.136 | 16.430 | 1.00 | 19.53 | 6 |
| | ATOM | 2394 | C | VAL | B | 27 | 59.576 | -7.694 | 15.308 | 1.00 | 21.55 | 6 |
| 60 | ATOM | 2395 | O | VAL | B | 27 | 60.170 | -8.516 | 14.520 | 1.00 | 22.20 | 8 |
| | ATOM | 2396 | CB | VAL | B | 27 | 59.378 | -9.239 | 17.253 | 1.00 | 21.88 | 6 |
| | ATOM | 2397 | CG1 | VAL | B | 27 | 60.658 | -8.617 | 17.884 | 1.00 | 21.20 | 6 |
| | ATOM | 2398 | CG2 | VAL | B | 27 | 58.513 | -9.837 | 18.318 | 1.00 | 20.54 | 6 |
| | ATOM | 2399 | N | PRO | B | 28 | 59.761 | -6.435 | 14.910 | 1.00 | 20.58 | 7 |
| 65 | ATOM | 2400 | CA | PRO | B | 28 | 60.557 | -5.881 | 13.878 | 1.00 | 21.31 | 6 |
| | ATOM | 2401 | C | PRO | B | 28 | 62.068 | -5.886 | 14.202 | 1.00 | 24.78 | 6 |
| | ATOM | 2402 | O | PRO | B | 28 | 62.428 | -5.538 | 15.336 | 1.00 | 26.50 | 8 |
| | ATOM | 2403 | CB | PRO | B | 28 | 60.112 | -4.424 | 13.720 | 1.00 | 22.66 | 6 |
| | ATOM | 2404 | CG | PRO | B | 28 | 58.741 | -4.426 | 14.395 | 1.00 | 20.85 | 6 |
| 70 | ATOM | 2405 | CD | PRO | B | 28 | 58.946 | -5.327 | 15.578 | 1.00 | 20.40 | 6 |
| | ATOM | 2406 | N | THR | B | 29 | 62.875 | -6.483 | 13.317 | 1.00 | 26.26 | 7 |
| | ATOM | 2407 | CA | THR | B | 29 | 64.329 | -6.556 | 13.614 | 1.00 | 25.08 | 6 |
| | ATOM | 2408 | C | THR | B | 29 | 65.126 | -6.328 | 12.359 | 1.00 | 25.98 | 6 |
| | ATOM | 2409 | O | THR | B | 29 | 64.643 | -6.415 | 11.228 | 1.00 | 23.47 | 8 |
| | ATOM | 2410 | CB | THR | B | 29 | 64.820 | -7.900 | 14.201 | 1.00 | 26.97 | 6 |

-69-

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|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|----|
| | ATOM | 2411 | OG1 | THR | B | 29 | 65.022 | -8.817 | 13.088 | 1.00 | 26.74 | 8 |
| | ATOM | 2412 | CG2 | THR | B | 29 | 63.914 | -8.579 | 15.219 | 1.00 | 25.95 | 6 |
| | ATOM | 2413 | N | MET | B | 30 | 66.471 | -6.078 | 12.560 | 1.00 | 25.32 | 7 |
| 5 | ATOM | 2414 | CA | MET | B | 30 | 67.357 | -5.995 | 11.415 | 1.00 | 26.82 | 6 |
| | ATOM | 2415 | C | MET | B | 30 | 68.261 | -7.249 | 11.384 | 1.00 | 28.96 | 6 |
| | ATOM | 2416 | O | MET | B | 30 | 69.347 | -7.183 | 10.815 | 1.00 | 30.56 | 8 |
| | ATOM | 2417 | CB | MET | B | 30 | 68.229 | -4.738 | 11.416 | 1.00 | 26.43 | 6 |
| | ATOM | 2418 | CG | MET | B | 30 | 67.252 | -3.504 | 11.203 | 1.00 | 27.24 | 6 |
| 10 | ATOM | 2419 | SD | MET | B | 30 | 67.969 | -2.187 | 10.263 | 1.00 | 28.19 | 16 |
| | ATOM | 2420 | CE | MET | B | 30 | 69.323 | -1.713 | 11.388 | 1.00 | 33.08 | 6 |
| | ATOM | 2421 | N | GLY | B | 31 | 67.793 | -8.340 | 11.934 | 1.00 | 27.82 | 7 |
| | ATOM | 2422 | CA | GLY | B | 31 | 68.599 | -9.593 | 11.926 | 1.00 | 29.40 | 6 |
| | ATOM | 2423 | C | GLY | B | 31 | 69.833 | -9.495 | 12.829 | 1.00 | 31.29 | 6 |
| 15 | ATOM | 2424 | O | GLY | B | 31 | 69.934 | -8.645 | 13.713 | 1.00 | 28.83 | 8 |
| | ATOM | 2425 | N | ASN | B | 32 | 70.728 | -10.486 | 12.690 | 1.00 | 31.40 | 7 |
| | ATOM | 2426 | CA | ASN | B | 32 | 71.923 | -10.565 | 13.552 | 1.00 | 33.60 | 6 |
| | ATOM | 2427 | C | ASN | B | 32 | 71.454 | -10.664 | 14.982 | 1.00 | 30.00 | 6 |
| | ATOM | 2428 | O | ASN | B | 32 | 71.870 | -9.961 | 15.906 | 1.00 | 32.23 | 8 |
| 20 | ATOM | 2429 | CB | ASN | B | 32 | 72.857 | -9.379 | 13.347 | 1.00 | 35.71 | 6 |
| | ATOM | 2430 | CG | ASN | B | 32 | 74.231 | -9.610 | 13.979 | 1.00 | 39.99 | 6 |
| | ATOM | 2431 | OD1 | ASN | B | 32 | 74.920 | -8.633 | 14.294 | 1.00 | 42.85 | 8 |
| | ATOM | 2432 | ND2 | ASN | B | 32 | 74.607 | -10.864 | 14.228 | 1.00 | 40.08 | 7 |
| | ATOM | 2433 | N | LEU | B | 33 | 70.506 | -11.572 | 15.191 | 1.00 | 30.19 | 7 |
| 25 | ATOM | 2434 | CA | LEU | B | 33 | 69.833 | -11.774 | 16.449 | 1.00 | 29.02 | 6 |
| | ATOM | 2435 | C | LEU | B | 33 | 70.684 | -12.343 | 17.566 | 1.00 | 35.03 | 6 |
| | ATOM | 2436 | O | LEU | B | 33 | 71.521 | -13.207 | 17.312 | 1.00 | 36.34 | 8 |
| | ATOM | 2437 | CB | LEU | B | 33 | 68.616 | -12.717 | 16.279 | 1.00 | 30.07 | 6 |
| | ATOM | 2438 | CG | LEU | B | 33 | 67.670 | -12.217 | 15.191 | 1.00 | 29.98 | 6 |
| 30 | ATOM | 2439 | CD1 | LEU | B | 33 | 66.434 | -13.121 | 15.083 | 1.00 | 31.08 | 6 |
| | ATOM | 2440 | CD2 | LEU | B | 33 | 67.221 | -10.777 | 15.431 | 1.00 | 28.84 | 6 |
| | ATOM | 2441 | N | HIS | B | 34 | 70.295 | -11.945 | 18.774 | 1.00 | 35.85 | 7 |
| | ATOM | 2442 | CA | HIS | B | 34 | 71.004 | -12.381 | 19.965 | 1.00 | 39.05 | 6 |
| | ATOM | 2443 | C | HIS | B | 34 | 69.976 | -12.567 | 21.067 | 1.00 | 37.94 | 6 |
| 35 | ATOM | 2444 | O | HIS | B | 34 | 68.762 | -12.451 | 20.791 | 1.00 | 37.26 | 8 |
| | ATOM | 2445 | CB | HIS | B | 34 | 72.097 | -11.404 | 20.404 | 1.00 | 40.15 | 6 |
| | ATOM | 2446 | CG | HIS | B | 34 | 71.668 | -10.006 | 20.714 | 1.00 | 42.43 | 6 |
| | ATOM | 2447 | ND1 | HIS | B | 34 | 70.876 | -9.671 | 21.799 | 1.00 | 44.12 | 7 |
| | ATOM | 2448 | CD2 | HIS | B | 34 | 71.953 | -8.848 | 20.062 | 1.00 | 43.13 | 6 |
| 40 | ATOM | 2449 | CE1 | HIS | B | 34 | 70.689 | -8.360 | 21.808 | 1.00 | 44.28 | 6 |
| | ATOM | 2450 | NE2 | HIS | B | 34 | 71.323 | -7.840 | 20.763 | 1.00 | 44.67 | 7 |
| | ATOM | 2451 | N | ASP | B | 35 | 70.439 | -12.874 | 22.263 | 1.00 | 36.30 | 7 |
| | ATOM | 2452 | CA | ASP | B | 35 | 69.531 | -13.176 | 23.352 | 1.00 | 38.71 | 6 |
| | ATOM | 2453 | C | ASP | B | 35 | 68.539 | -12.055 | 23.649 | 1.00 | 38.11 | 6 |
| 45 | ATOM | 2454 | O | ASP | B | 35 | 67.448 | -12.373 | 24.116 | 1.00 | 38.15 | 8 |
| | ATOM | 2455 | CB | ASP | B | 35 | 70.309 | -13.480 | 24.637 | 1.00 | 43.89 | 6 |
| | ATOM | 2456 | CG | ASP | B | 35 | 71.071 | -14.776 | 24.631 | 1.00 | 48.19 | 6 |
| | ATOM | 2457 | OD1 | ASP | B | 35 | 71.046 | -15.496 | 23.603 | 1.00 | 50.75 | 8 |
| | ATOM | 2458 | OD2 | ASP | B | 35 | 71.701 | -15.074 | 25.689 | 1.00 | 51.91 | 8 |
| 50 | ATOM | 2459 | N | GLY | B | 36 | 68.919 | -10.788 | 23.499 | 1.00 | 35.59 | 7 |
| | ATOM | 2460 | CA | GLY | B | 36 | 68.007 | -9.688 | 23.778 | 1.00 | 33.96 | 6 |
| | ATOM | 2461 | C | GLY | B | 36 | 66.844 | -9.774 | 22.751 | 1.00 | 32.11 | 6 |
| | ATOM | 2462 | O | GLY | B | 36 | 65.738 | -9.524 | 23.235 | 1.00 | 30.98 | 8 |
| | ATOM | 2463 | N | HIS | B | 37 | 67.149 | -10.177 | 21.521 | 1.00 | 31.48 | 7 |
| 55 | ATOM | 2464 | CA | HIS | B | 37 | 66.006 | -10.322 | 20.581 | 1.00 | 31.68 | 6 |
| | ATOM | 2465 | C | HIS | B | 37 | 65.118 | -11.479 | 20.969 | 1.00 | 33.06 | 6 |
| | ATOM | 2466 | O | HIS | B | 37 | 63.861 | -11.440 | 20.850 | 1.00 | 30.99 | 8 |
| | ATOM | 2467 | CB | HIS | B | 37 | 66.507 | -10.514 | 19.175 | 1.00 | 31.96 | 6 |
| | ATOM | 2468 | CG | HIS | B | 37 | 67.366 | -9.425 | 18.643 | 1.00 | 34.37 | 6 |
| 60 | ATOM | 2469 | ND1 | HIS | B | 37 | 66.888 | -8.299 | 18.005 | 1.00 | 37.43 | 7 |
| | ATOM | 2470 | CD2 | HIS | B | 37 | 68.714 | -9.330 | 18.624 | 1.00 | 34.96 | 6 |
| | ATOM | 2471 | CE1 | HIS | B | 37 | 67.890 | -7.535 | 17.580 | 1.00 | 35.54 | 6 |
| | ATOM | 2472 | NE2 | HIS | B | 37 | 69.003 | -8.153 | 17.962 | 1.00 | 39.23 | 7 |
| | ATOM | 2473 | N | MET | B | 38 | 65.704 | -12.577 | 21.486 | 1.00 | 31.32 | 7 |
| 65 | ATOM | 2474 | CA | MET | B | 38 | 64.880 | -13.668 | 22.001 | 1.00 | 31.44 | 6 |
| | ATOM | 2475 | C | MET | B | 38 | 63.959 | -13.252 | 23.115 | 1.00 | 29.66 | 6 |
| | ATOM | 2476 | O | MET | B | 38 | 62.851 | -13.809 | 23.253 | 1.00 | 28.40 | 8 |
| | ATOM | 2477 | CB | MET | B | 38 | 65.799 | -14.827 | 21.487 | 1.00 | 34.21 | 6 |
| | ATOM | 2478 | CG | MET | B | 38 | 66.423 | -15.620 | 21.375 | 1.00 | 35.15 | 6 |
| 70 | ATOM | 2479 | SD | MET | B | 38 | 65.631 | -15.970 | 19.832 | 1.00 | 35.12 | 16 |
| | ATOM | 2480 | CE | MET | B | 38 | 66.123 | -14.628 | 18.770 | 1.00 | 36.33 | 6 |
| | ATOM | 2481 | N | LYS | B | 39 | 64.228 | -12.300 | 23.996 | 1.00 | 29.09 | 7 |
| | ATOM | 2482 | CA | LYS | B | 39 | 63.368 | -11.857 | 25.065 | 1.00 | 26.18 | 6 |
| | ATOM | 2483 | C | LYS | B | 39 | 62.142 | -11.078 | 24.470 | 1.00 | 25.41 | 6 |
| | ATOM | 2484 | O | LYS | B | 39 | 61.042 | -11.228 | 24.964 | 1.00 | 26.08 | 8 |

-70-

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|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| | ATOM | 2485 | CB | LYS | B | 39 | 64.048 | -10.935 | 26.076 | 1.00 | 27.75 | 6 |
| | ATOM | 2486 | CG | LYS | B | 39 | 63.195 | -10.551 | 27.262 | 1.00 | 27.45 | 6 |
| | ATOM | 2487 | CD | LYS | B | 39 | 64.031 | -9.643 | 28.216 | 1.00 | 30.13 | 6 |
| 5 | ATOM | 2488 | CE | LYS | B | 39 | 63.142 | -9.261 | 29.377 | 1.00 | 29.21 | 6 |
| | ATOM | 2489 | NZ | LYS | B | 39 | 63.883 | -8.413 | 30.361 | 1.00 | 32.36 | 7 |
| | ATOM | 2490 | N | LEU | B | 40 | 62.394 | -10.379 | 23.402 | 1.00 | 26.07 | 7 |
| | ATOM | 2491 | CA | LEU | B | 40 | 61.256 | -9.741 | 22.709 | 1.00 | 25.52 | 6 |
| | ATOM | 2492 | C | LEU | B | 40 | 60.254 | -10.805 | 22.220 | 1.00 | 25.72 | 6 |
| 10 | ATOM | 2493 | O | LEU | B | 40 | 59.055 | -10.609 | 22.293 | 1.00 | 23.50 | 8 |
| | ATOM | 2494 | CB | LEU | B | 40 | 61.702 | -8.954 | 21.497 | 1.00 | 26.47 | 6 |
| | ATOM | 2495 | CG | LEU | B | 40 | 62.739 | -7.859 | 21.758 | 1.00 | 30.07 | 6 |
| | ATOM | 2496 | CD1 | LEU | B | 40 | 63.073 | -7.128 | 20.474 | 1.00 | 31.00 | 6 |
| | ATOM | 2497 | CD2 | LEU | B | 40 | 62.237 | -6.905 | 22.832 | 1.00 | 30.41 | 6 |
| 15 | ATOM | 2498 | N | VAL | B | 41 | 60.844 | -11.842 | 21.611 | 1.00 | 25.04 | 7 |
| | ATOM | 2499 | CA | VAL | B | 41 | 59.995 | -12.936 | 21.065 | 1.00 | 24.43 | 6 |
| | ATOM | 2500 | C | VAL | B | 41 | 59.235 | -13.579 | 22.162 | 1.00 | 23.84 | 6 |
| | ATOM | 2501 | O | VAL | B | 41 | 58.037 | -13.868 | 22.103 | 1.00 | 23.75 | 8 |
| | ATOM | 2502 | CB | VAL | B | 41 | 60.893 | -13.922 | 20.289 | 1.00 | 24.40 | 6 |
| 20 | ATOM | 2503 | CG1 | VAL | B | 41 | 60.057 | -15.140 | 19.914 | 1.00 | 24.57 | 6 |
| | ATOM | 2504 | CG2 | VAL | B | 41 | 61.496 | -13.337 | 19.019 | 1.00 | 25.66 | 6 |
| | ATOM | 2505 | N | ASP | B | 42 | 59.826 | -13.850 | 23.376 | 1.00 | 25.85 | 7 |
| | ATOM | 2506 | CA | ASP | B | 42 | 59.130 | -14.426 | 24.480 | 1.00 | 26.19 | 6 |
| | ATOM | 2507 | C | ASP | B | 42 | 57.994 | -13.543 | 24.981 | 1.00 | 28.20 | 6 |
| 25 | ATOM | 2508 | O | ASP | B | 42 | 56.910 | -14.030 | 25.341 | 1.00 | 27.55 | 8 |
| | ATOM | 2509 | CB | ASP | B | 42 | 60.131 | -14.709 | 25.659 | 1.00 | 29.50 | 6 |
| | ATOM | 2510 | CG | ASP | B | 42 | 61.118 | -15.822 | 25.377 | 1.00 | 32.71 | 6 |
| | ATOM | 2511 | OD1 | ASP | B | 42 | 61.051 | -16.616 | 24.419 | 1.00 | 33.03 | 8 |
| | ATOM | 2512 | OD2 | ASP | B | 42 | 62.135 | -15.893 | 26.160 | 1.00 | 33.67 | 8 |
| 30 | ATOM | 2513 | N | GLU | B | 43 | 58.205 | -12.216 | 24.957 | 1.00 | 26.23 | 7 |
| | ATOM | 2514 | CA | GLU | B | 43 | 57.130 | -11.321 | 25.355 | 1.00 | 27.21 | 6 |
| | ATOM | 2515 | C | GLU | B | 43 | 55.973 | -11.339 | 24.327 | 1.00 | 24.30 | 6 |
| | ATOM | 2516 | O | GLU | B | 43 | 54.809 | -11.340 | 24.709 | 1.00 | 24.66 | 8 |
| | ATOM | 2517 | CB | GLU | B | 43 | 57.676 | -9.912 | 25.475 | 1.00 | 30.67 | 6 |
| 35 | ATOM | 2518 | CG | GLU | B | 43 | 56.740 | -8.904 | 26.130 | 1.00 | 36.81 | 6 |
| | ATOM | 2519 | CD | GLU | B | 43 | 56.445 | -9.257 | 27.585 | 1.00 | 40.25 | 6 |
| | ATOM | 2520 | OE1 | GLU | B | 43 | 57.347 | -9.847 | 28.236 | 1.00 | 44.07 | 8 |
| | ATOM | 2521 | OE2 | GLU | B | 43 | 55.348 | -8.999 | 28.121 | 1.00 | 40.92 | 8 |
| | ATOM | 2522 | N | ALA | B | 44 | 56.324 | -11.466 | 23.083 | 1.00 | 26.35 | 7 |
| 40 | ATOM | 2523 | CA | ALA | B | 44 | 55.321 | -11.474 | 21.969 | 1.00 | 23.41 | 6 |
| | ATOM | 2524 | C | ALA | B | 44 | 54.526 | -12.754 | 22.079 | 1.00 | 26.63 | 6 |
| | ATOM | 2525 | O | ALA | B | 44 | 53.287 | -12.728 | 22.074 | 1.00 | 26.61 | 8 |
| | ATOM | 2526 | CB | ALA | B | 44 | 56.007 | -11.299 | 20.651 | 1.00 | 25.41 | 6 |
| | ATOM | 2527 | N | LYS | B | 45 | 55.209 | -13.882 | 22.329 | 1.00 | 27.34 | 7 |
| 45 | ATOM | 2528 | CA | LYS | B | 45 | 54.542 | -15.169 | 22.501 | 1.00 | 29.71 | 6 |
| | ATOM | 2529 | C | LYS | B | 45 | 53.589 | -15.160 | 23.659 | 1.00 | 28.45 | 6 |
| | ATOM | 2530 | O | LYS | B | 45 | 52.559 | -15.805 | 23.717 | 1.00 | 28.18 | 8 |
| | ATOM | 2531 | CB | LYS | B | 45 | 55.537 | -16.322 | 22.783 | 1.00 | 32.90 | 6 |
| | ATOM | 2532 | CG | LYS | B | 45 | 56.368 | -16.726 | 21.588 | 1.00 | 38.80 | 6 |
| 50 | ATOM | 2533 | CD | LYS | B | 45 | 57.724 | -17.301 | 21.961 | 1.00 | 43.49 | 6 |
| | ATOM | 2534 | CE | LYS | B | 45 | 57.757 | -18.398 | 23.004 | 1.00 | 46.00 | 6 |
| | ATOM | 2535 | NZ | LYS | B | 45 | 59.077 | -18.396 | 23.727 | 1.00 | 47.62 | 7 |
| | ATOM | 2536 | N | ALA | B | 46 | 53.935 | -14.446 | 24.748 | 1.00 | 27.58 | 7 |
| | ATOM | 2537 | CA | ALA | B | 46 | 53.076 | -14.389 | 25.900 | 1.00 | 27.60 | 6 |
| 55 | ATOM | 2538 | C | ALA | B | 46 | 51.831 | -13.527 | 25.751 | 1.00 | 28.91 | 6 |
| | ATOM | 2539 | O | ALA | B | 46 | 50.905 | -13.633 | 26.549 | 1.00 | 30.19 | 8 |
| | ATOM | 2540 | CB | ALA | B | 46 | 53.882 | -13.818 | 27.097 | 1.00 | 28.29 | 6 |
| | ATOM | 2541 | N | ARG | B | 47 | 51.754 | -12.657 | 24.741 | 1.00 | 26.88 | 7 |
| | ATOM | 2542 | CA | ARG | B | 47 | 50.691 | -11.719 | 24.586 | 1.00 | 25.76 | 6 |
| 60 | ATOM | 2543 | C | ARG | B | 47 | 49.781 | -11.972 | 23.373 | 1.00 | 23.01 | 6 |
| | ATOM | 2544 | O | ARG | B | 47 | 48.813 | -11.243 | 23.291 | 1.00 | 23.89 | 8 |
| | ATOM | 2545 | CB | ARG | B | 47 | 51.345 | -10.312 | 24.433 | 1.00 | 24.92 | 6 |
| | ATOM | 2546 | CG | ARG | B | 47 | 51.975 | -9.858 | 25.800 | 1.00 | 27.22 | 6 |
| | ATOM | 2547 | CD | ARG | B | 47 | 52.755 | -8.575 | 25.491 | 1.00 | 29.69 | 6 |
| 65 | ATOM | 2548 | NE | ARG | B | 47 | 53.415 | -7.966 | 26.670 | 1.00 | 34.33 | 7 |
| | ATOM | 2549 | CZ | ARG | B | 47 | 52.861 | -6.966 | 27.358 | 1.00 | 35.85 | 6 |
| | ATOM | 2550 | NH1 | ARG | B | 47 | 51.680 | -6.442 | 27.073 | 1.00 | 35.22 | 7 |
| | ATOM | 2551 | NH2 | ARG | B | 47 | 53.555 | -6.467 | 28.392 | 1.00 | 37.54 | 7 |
| | ATOM | 2552 | N | ALA | B | 48 | 50.203 | -12.899 | 22.529 | 1.00 | 23.33 | 7 |
| 70 | ATOM | 2553 | CA | ALA | B | 48 | 49.413 | -13.114 | 21.284 | 1.00 | 23.32 | 6 |
| | ATOM | 2554 | C | ALA | B | 48 | 49.405 | -14.574 | 20.933 | 1.00 | 26.45 | 6 |
| | ATOM | 2555 | O | ALA | B | 48 | 50.224 | -15.356 | 21.466 | 1.00 | 24.59 | 8 |
| | ATOM | 2556 | CB | ALA | B | 48 | 50.059 | -12.332 | 20.168 | 1.00 | 23.24 | 6 |
| | ATOM | 2557 | N | ASP | B | 49 | 48.547 | -15.010 | 20.004 | 1.00 | 24.54 | 7 |
| | ATOM | 2558 | CA | ASP | B | 49 | 48.537 | -16.394 | 19.594 | 1.00 | 24.90 | 6 |

-71-

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|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| | ATOM | 2559 | C | ASP | B | 49 | 49.677 | -16.770 | 18.689 | 1.00 | 24.42 | 6 |
| | ATOM | 2560 | O | ASP | B | 49 | 50.254 | -17.869 | 18.668 | 1.00 | 26.07 | 8 |
| | ATOM | 2561 | CB | ASP | B | 49 | 47.237 | -16.656 | 18.803 | 1.00 | 26.28 | 6 |
| 5 | ATOM | 2562 | CG | ASP | B | 49 | 45.979 | -16.417 | 19.627 | 1.00 | 30.04 | 6 |
| | ATOM | 2563 | OD1 | ASP | B | 49 | 45.977 | -16.990 | 20.754 | 1.00 | 32.57 | 8 |
| | ATOM | 2564 | OD2 | ASP | B | 49 | 45.038 | -15.712 | 19.183 | 1.00 | 30.75 | 8 |
| | ATOM | 2565 | N | VAL | B | 50 | 50.004 | -15.842 | 17.792 | 1.00 | 20.95 | 7 |
| | ATOM | 2566 | CA | VAL | B | 50 | 50.980 | -15.998 | 16.747 | 1.00 | 20.87 | 6 |
| 10 | ATOM | 2567 | C | VAL | B | 50 | 52.014 | -14.905 | 16.734 | 1.00 | 20.83 | 6 |
| | ATOM | 2568 | O | VAL | B | 50 | 51.742 | -13.704 | 16.973 | 1.00 | 20.70 | 8 |
| | ATOM | 2569 | CB | VAL | B | 50 | 50.241 | -16.031 | 15.369 | 1.00 | 22.53 | 6 |
| | ATOM | 2570 | CG1 | VAL | B | 50 | 51.112 | -15.780 | 14.170 | 1.00 | 26.09 | 6 |
| | ATOM | 2571 | CG2 | VAL | B | 50 | 49.536 | -17.393 | 15.199 | 1.00 | 25.40 | 6 |
| 15 | ATOM | 2572 | N | VAL | B | 51 | 53.286 | -15.325 | 16.567 | 1.00 | 19.42 | 7 |
| | ATOM | 2573 | CA | VAL | B | 51 | 54.373 | -14.336 | 16.498 | 1.00 | 22.20 | 6 |
| | ATOM | 2574 | C | VAL | B | 51 | 54.975 | -14.279 | 15.113 | 1.00 | 22.35 | 6 |
| | ATOM | 2575 | O | VAL | B | 51 | 55.400 | -15.274 | 14.488 | 1.00 | 23.37 | 8 |
| | ATOM | 2576 | CB | VAL | B | 51 | 55.498 | -14.618 | 17.516 | 1.00 | 23.80 | 6 |
| 20 | ATOM | 2577 | CG1 | VAL | B | 51 | 56.616 | -13.574 | 17.449 | 1.00 | 24.48 | 6 |
| | ATOM | 2578 | CG2 | VAL | B | 51 | 54.855 | -14.682 | 18.910 | 1.00 | 28.00 | 6 |
| | ATOM | 2579 | N | VAL | B | 52 | 55.108 | -13.080 | 14.590 | 1.00 | 18.68 | 7 |
| | ATOM | 2580 | CA | VAL | B | 52 | 55.734 | -12.772 | 13.322 | 1.00 | 17.55 | 6 |
| | ATOM | 2581 | C | VAL | B | 52 | 57.014 | -11.980 | 13.623 | 1.00 | 21.15 | 6 |
| 25 | ATOM | 2582 | O | VAL | B | 52 | 56.930 | -10.957 | 14.319 | 1.00 | 19.41 | 8 |
| | ATOM | 2583 | CB | VAL | B | 52 | 54.885 | -11.936 | 12.341 | 1.00 | 19.87 | 6 |
| | ATOM | 2584 | CG1 | VAL | B | 52 | 55.613 | -11.467 | 11.107 | 1.00 | 19.90 | 6 |
| | ATOM | 2585 | CG2 | VAL | B | 52 | 53.651 | -12.759 | 11.943 | 1.00 | 20.31 | 6 |
| | ATOM | 2586 | N | VAL | B | 53 | 58.150 | -12.469 | 13.104 | 1.00 | 20.72 | 7 |
| 30 | ATOM | 2587 | CA | VAL | B | 53 | 59.396 | -11.698 | 13.267 | 1.00 | 20.35 | 6 |
| | ATOM | 2588 | C | VAL | B | 53 | 59.854 | -11.261 | 11.925 | 1.00 | 22.26 | 6 |
| | ATOM | 2589 | O | VAL | B | 53 | 59.933 | -12.026 | 10.948 | 1.00 | 23.47 | 8 |
| | ATOM | 2590 | CB | VAL | B | 53 | 60.505 | -12.545 | 13.977 | 1.00 | 20.44 | 6 |
| | ATOM | 2591 | CG1 | VAL | B | 53 | 61.791 | -11.700 | 14.053 | 1.00 | 22.35 | 6 |
| 35 | ATOM | 2592 | CG2 | VAL | B | 53 | 60.059 | -13.004 | 15.346 | 1.00 | 22.26 | 6 |
| | ATOM | 2593 | N | SER | B | 54 | 60.144 | -9.957 | 11.694 | 1.00 | 20.14 | 7 |
| | ATOM | 2594 | CA | SER | B | 54 | 60.629 | -9.453 | 10.425 | 1.00 | 20.53 | 6 |
| | ATOM | 2595 | C | SER | B | 54 | 62.157 | -9.208 | 10.601 | 1.00 | 23.03 | 6 |
| | ATOM | 2596 | O | SER | B | 54 | 62.594 | -8.867 | 11.697 | 1.00 | 23.22 | 8 |
| 40 | ATOM | 2597 | CB | SER | B | 54 | 59.973 | -8.182 | 9.883 | 1.00 | 24.56 | 6 |
| | ATOM | 2598 | OG | SER | B | 54 | 60.079 | -7.161 | 10.861 | 1.00 | 24.52 | 8 |
| | ATOM | 2599 | N | ILE | B | 55 | 62.804 | -9.615 | 9.537 | 1.00 | 25.11 | 7 |
| | ATOM | 2600 | CA | ILE | B | 55 | 64.289 | -9.443 | 9.508 | 1.00 | 23.93 | 6 |
| | ATOM | 2601 | C | ILE | B | 55 | 64.589 | -8.756 | 8.220 | 1.00 | 22.42 | 6 |
| 45 | ATOM | 2602 | O | ILE | B | 55 | 64.333 | -9.214 | 7.082 | 1.00 | 23.75 | 8 |
| | ATOM | 2603 | CB | ILE | B | 55 | 65.017 | -10.788 | 9.599 | 1.00 | 25.95 | 6 |
| | ATOM | 2604 | CG1 | ILE | B | 55 | 64.888 | -11.494 | 10.920 | 1.00 | 25.74 | 6 |
| | ATOM | 2605 | CG2 | ILE | B | 55 | 66.512 | -10.480 | 9.307 | 1.00 | 26.43 | 6 |
| | ATOM | 2606 | CD1 | ILE | B | 55 | 65.315 | -12.955 | 10.805 | 1.00 | 29.38 | 6 |
| 50 | ATOM | 2607 | N | PHE | B | 56 | 65.039 | -7.469 | 8.273 | 1.00 | 23.02 | 7 |
| | ATOM | 2608 | CA | PHE | B | 56 | 65.225 | -6.624 | 7.153 | 1.00 | 24.66 | 6 |
| | ATOM | 2609 | C | PHE | B | 56 | 66.202 | -5.465 | 7.454 | 1.00 | 26.79 | 6 |
| | ATOM | 2610 | O | PHE | B | 56 | 65.937 | -4.712 | 8.392 | 1.00 | 26.50 | 8 |
| | ATOM | 2611 | CB | PHE | B | 56 | 63.878 | -6.011 | 6.668 | 1.00 | 22.93 | 6 |
| 55 | ATOM | 2612 | CG | PHE | B | 56 | 64.081 | -5.130 | 5.476 | 1.00 | 24.37 | 6 |
| | ATOM | 2613 | CD1 | PHE | B | 56 | 64.570 | -5.602 | 4.262 | 1.00 | 25.67 | 6 |
| | ATOM | 2614 | CD2 | PHE | B | 56 | 63.711 | -3.781 | 5.549 | 1.00 | 23.80 | 6 |
| | ATOM | 2615 | CE1 | PHE | B | 56 | 64.765 | -4.758 | 3.193 | 1.00 | 25.30 | 6 |
| | ATOM | 2616 | CE2 | PHE | B | 56 | 63.882 | -2.969 | 4.441 | 1.00 | 25.84 | 6 |
| 60 | ATOM | 2617 | CZ | PHE | B | 56 | 64.399 | -3.429 | 3.249 | 1.00 | 27.27 | 6 |
| | ATOM | 2618 | N | VAL | B | 57 | 67.330 | -5.512 | 6.717 | 1.00 | 28.13 | 7 |
| | ATOM | 2619 | CA | VAL | B | 57 | 68.347 | -4.471 | 7.001 | 1.00 | 27.59 | 6 |
| | ATOM | 2620 | C | VAL | B | 57 | 67.968 | -3.357 | 6.089 | 1.00 | 26.50 | 6 |
| | ATOM | 2621 | O | VAL | B | 57 | 68.047 | -3.404 | 4.871 | 1.00 | 28.47 | 8 |
| 65 | ATOM | 2622 | CB | VAL | B | 57 | 69.787 | -5.034 | 6.846 | 1.00 | 28.54 | 6 |
| | ATOM | 2623 | CG1 | VAL | B | 57 | 70.795 | -3.915 | 7.235 | 1.00 | 30.14 | 6 |
| | ATOM | 2624 | CG2 | VAL | B | 57 | 70.028 | -6.232 | 7.674 | 1.00 | 27.80 | 6 |
| | ATOM | 2625 | N | ASN | B | 58 | 67.280 | -2.367 | 6.723 | 1.00 | 27.33 | 7 |
| | ATOM | 2626 | CA | ASN | B | 58 | 66.643 | -1.277 | 5.989 | 1.00 | 28.47 | 6 |
| 70 | ATOM | 2627 | C | ASN | B | 58 | 67.589 | -0.208 | 5.529 | 1.00 | 28.30 | 6 |
| | ATOM | 2628 | O | ASN | B | 58 | 68.068 | 0.587 | 6.350 | 1.00 | 29.87 | 8 |
| | ATOM | 2629 | CB | ASN | B | 58 | 65.608 | -0.711 | 7.004 | 1.00 | 27.68 | 6 |
| | ATOM | 2630 | CG | ASN | B | 58 | 64.919 | 0.542 | 6.507 | 1.00 | 24.26 | 6 |
| | ATOM | 2631 | OD1 | ASN | B | 58 | 64.739 | 0.717 | 5.301 | 1.00 | 26.55 | 8 |
| | ATOM | 2632 | ND2 | ASN | B | 58 | 64.487 | 1.392 | 7.445 | 1.00 | 24.78 | 7 |

-72-

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|----|------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| | ATOM | 2633 | N | PRO | B | 59 | 67.828 | -0.063 | 4.251 | 1.00 | 32.20 | 7 |
| | ATOM | 2634 | CA | PRO | B | 59 | 68.766 | 0.929 | 3.749 | 1.00 | 32.85 | 6 |
| | ATOM | 2635 | C | PRO | B | 59 | 68.415 | 2.336 | 4.177 | 1.00 | 35.54 | 6 |
| 5 | ATOM | 2636 | O | PRO | B | 59 | 69.298 | 3.191 | 4.360 | 1.00 | 33.70 | 8 |
| | ATOM | 2637 | CB | PRO | B | 59 | 68.703 | 0.729 | 2.239 | 1.00 | 36.08 | 6 |
| | ATOM | 2638 | CG | PRO | B | 59 | 68.404 | -0.761 | 2.113 | 1.00 | 35.06 | 6 |
| | ATOM | 2639 | CD | PRO | B | 59 | 67.336 | -0.957 | 3.170 | 1.00 | 34.20 | 6 |
| | ATOM | 2640 | N | MET | B | 60 | 67.111 | 2.642 | 4.360 | 1.00 | 34.39 | 7 |
| 10 | ATOM | 2641 | CA | MET | B | 60 | 66.683 | 3.994 | 4.699 | 1.00 | 36.32 | 6 |
| | ATOM | 2642 | C | MET | B | 60 | 67.197 | 4.523 | 6.022 | 1.00 | 37.35 | 6 |
| | ATOM | 2643 | O | MET | B | 60 | 67.169 | 5.772 | 6.239 | 1.00 | 38.05 | 8 |
| | ATOM | 2644 | CB | MET | B | 60 | 65.148 | 4.088 | 4.790 | 1.00 | 37.91 | 6 |
| | ATOM | 2645 | CG | MET | B | 60 | 64.450 | 4.720 | 3.624 | 1.00 | 39.92 | 6 |
| 15 | ATOM | 2646 | SD | MET | B | 60 | 62.934 | 5.666 | 4.060 | 1.00 | 39.02 | 16 |
| | ATOM | 2647 | CE | MET | B | 60 | 61.890 | 5.076 | 2.719 | 1.00 | 40.24 | 6 |
| | ATOM | 2648 | N | GLN | B | 61 | 67.520 | 3.632 | 6.950 | 1.00 | 36.15 | 7 |
| | ATOM | 2649 | CA | GLN | B | 61 | 67.973 | 4.079 | 8.262 | 1.00 | 37.72 | 6 |
| | ATOM | 2650 | C | GLN | B | 61 | 69.493 | 3.884 | 8.375 | 1.00 | 39.87 | 6 |
| 20 | ATOM | 2651 | O | GLN | B | 61 | 70.042 | 3.727 | 9.476 | 1.00 | 42.79 | 8 |
| | ATOM | 2652 | CB | GLN | B | 61 | 67.179 | 3.390 | 9.361 | 1.00 | 35.80 | 6 |
| | ATOM | 2653 | CG | GLN | B | 61 | 67.540 | 1.949 | 9.681 | 1.00 | 32.41 | 6 |
| | ATOM | 2654 | CD | GLN | B | 61 | 66.514 | 1.303 | 10.572 | 1.00 | 29.81 | 6 |
| | ATOM | 2655 | OE1 | GLN | B | 61 | 65.349 | 0.972 | 10.194 | 1.00 | 28.50 | 8 |
| 25 | ATOM | 2656 | NE2 | GLN | B | 61 | 66.860 | 0.939 | 11.787 | 1.00 | 27.42 | 7 |
| | ATOM | 2657 | N | PHE | B | 62 | 70.210 | 3.961 | 7.244 | 1.00 | 39.42 | 7 |
| | ATOM | 2658 | CA | PHE | B | 62 | 71.665 | 3.901 | 7.241 | 1.00 | 40.52 | 6 |
| | ATOM | 2659 | C | PHE | B | 62 | 72.216 | 5.205 | 6.643 | 1.00 | 43.48 | 6 |
| | ATOM | 2660 | O | PHE | B | 62 | 71.742 | 5.679 | 5.613 | 1.00 | 41.80 | 8 |
| 30 | ATOM | 2661 | CB | PHE | B | 62 | 72.285 | 2.727 | 6.462 | 1.00 | 39.44 | 6 |
| | ATOM | 2662 | CG | PHE | B | 62 | 72.261 | 1.476 | 7.310 | 1.00 | 38.25 | 6 |
| | ATOM | 2663 | CD1 | PHE | B | 62 | 71.094 | 0.697 | 7.350 | 1.00 | 37.73 | 6 |
| | ATOM | 2664 | CD2 | PHE | B | 62 | 73.329 | 1.085 | 8.076 | 1.00 | 37.32 | 6 |
| | ATOM | 2665 | CE1 | PHE | B | 62 | 71.053 | -0.422 | 8.157 | 1.00 | 37.14 | 6 |
| 35 | ATOM | 2666 | CE2 | PHE | B | 62 | 73.294 | -0.044 | 8.870 | 1.00 | 36.89 | 6 |
| | ATOM | 2667 | CZ | PHE | B | 62 | 72.145 | -0.825 | 8.902 | 1.00 | 37.49 | 6 |
| | ATOM | 2668 | N | ASP | B | 63 | 73.267 | 5.723 | 7.257 | 1.00 | 48.37 | 7 |
| | ATOM | 2669 | CA | ASP | B | 63 | 73.887 | 6.980 | 6.816 | 1.00 | 51.97 | 6 |
| | ATOM | 2670 | C | ASP | B | 63 | 74.709 | 6.872 | 5.539 | 1.00 | 53.02 | 6 |
| 40 | ATOM | 2671 | O | ASP | B | 63 | 74.642 | 7.765 | 4.679 | 1.00 | 53.58 | 8 |
| | ATOM | 2672 | CB | ASP | B | 63 | 74.800 | 7.511 | 7.922 | 1.00 | 53.54 | 6 |
| | ATOM | 2673 | CG | ASP | B | 63 | 74.087 | 7.668 | 9.251 | 1.00 | 55.47 | 6 |
| | ATOM | 2674 | OD1 | ASP | B | 63 | 72.832 | 7.712 | 9.265 | 1.00 | 57.99 | 8 |
| | ATOM | 2675 | OD2 | ASP | B | 63 | 74.767 | 7.751 | 10.294 | 1.00 | 56.33 | 8 |
| 45 | ATOM | 2676 | N | ARG | B | 64 | 75.521 | 5.830 | 5.420 | 1.00 | 52.77 | 7 |
| | ATOM | 2677 | CA | ARG | B | 64 | 76.344 | 5.697 | 4.211 | 1.00 | 54.08 | 6 |
| | ATOM | 2678 | C | ARG | B | 64 | 76.323 | 4.250 | 3.759 | 1.00 | 54.41 | 6 |
| | ATOM | 2679 | O | ARG | B | 64 | 76.037 | 3.392 | 4.582 | 1.00 | 53.32 | 8 |
| | ATOM | 2680 | CB | ARG | B | 64 | 77.758 | 6.205 | 4.486 | 1.00 | 53.78 | 6 |
| 50 | ATOM | 2681 | N | PRO | B | 65 | 76.658 | 3.987 | 2.505 | 1.00 | 56.79 | 7 |
| | ATOM | 2682 | CA | PRO | B | 65 | 76.654 | 2.637 | 1.974 | 1.00 | 57.90 | 6 |
| | ATOM | 2683 | C | PRO | B | 65 | 77.533 | 1.632 | 2.682 | 1.00 | 59.54 | 6 |
| | ATOM | 2684 | O | PRO | B | 65 | 77.159 | 0.456 | 2.659 | 1.00 | 59.29 | 8 |
| | ATOM | 2685 | CB | PRO | B | 65 | 77.123 | 2.790 | 0.528 | 1.00 | 58.01 | 6 |
| 55 | ATOM | 2686 | CG | PRO | B | 65 | 77.017 | 4.235 | 0.201 | 1.00 | 58.02 | 6 |
| | ATOM | 2687 | CD | PRO | B | 65 | 77.011 | 5.007 | 1.489 | 1.00 | 57.36 | 6 |
| | ATOM | 2688 | N | GLU | B | 66 | 78.651 | 1.990 | 3.291 | 1.00 | 60.73 | 7 |
| | ATOM | 2689 | CA | GLU | B | 66 | 79.545 | 1.029 | 3.926 | 1.00 | 60.74 | 6 |
| | ATOM | 2690 | C | GLU | B | 66 | 78.996 | 0.590 | 5.268 | 1.00 | 58.41 | 6 |
| 60 | ATOM | 2691 | O | GLU | B | 66 | 79.184 | -0.554 | 5.672 | 1.00 | 59.32 | 8 |
| | ATOM | 2692 | CB | GLU | B | 66 | 80.949 | 1.612 | 4.114 | 1.00 | 63.95 | 6 |
| | ATOM | 2693 | CG | GLU | B | 66 | 81.554 | 2.085 | 2.807 | 1.00 | 67.09 | 6 |
| | ATOM | 2694 | CD | GLU | B | 66 | 81.129 | 3.469 | 2.387 | 1.00 | 69.60 | 6 |
| | ATOM | 2695 | OE1 | GLU | B | 66 | 80.077 | 4.027 | 2.774 | 1.00 | 71.11 | 8 |
| 65 | ATOM | 2696 | OE2 | GLU | B | 66 | 81.873 | 4.122 | 1.612 | 1.00 | 71.37 | 8 |
| | ATOM | 2697 | N | ASP | B | 67 | 78.271 | 1.521 | 5.890 | 1.00 | 55.22 | 7 |
| | ATOM | 2698 | CA | ASP | B | 67 | 77.618 | 1.142 | 7.151 | 1.00 | 53.44 | 6 |
| | ATOM | 2699 | C | ASP | B | 67 | 76.586 | 0.068 | 6.773 | 1.00 | 49.67 | 6 |
| | ATOM | 2700 | O | ASP | B | 67 | 76.505 | -0.978 | 7.418 | 1.00 | 47.57 | 8 |
| 70 | ATOM | 2701 | CB | ASP | B | 67 | 77.109 | 2.400 | 7.818 | 1.00 | 55.45 | 6 |
| | ATOM | 2702 | CG | ASP | B | 67 | 78.226 | 3.389 | 8.134 | 1.00 | 58.05 | 6 |
| | ATOM | 2703 | OD1 | ASP | B | 67 | 79.352 | 3.283 | 7.602 | 1.00 | 58.16 | 8 |
| | ATOM | 2704 | OD2 | ASP | B | 67 | 77.993 | 4.307 | 8.954 | 1.00 | 58.74 | 8 |
| | ATOM | 2705 | N | LEU | B | 68 | 75.906 | 0.243 | 5.640 | 1.00 | 47.47 | 7 |
| | ATOM | 2706 | CA | LEU | B | 68 | 74.908 | -0.706 | 5.170 | 1.00 | 45.94 | 6 |

-73-

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|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| | ATOM | 2707 | C | LEU | B | 68 | 75.575 | -2.002 | 4.715 | 1.00 | 46.59 | 6 |
| | ATOM | 2708 | O | LEU | B | 68 | 75.241 | -3.082 | 5.201 | 1.00 | 47.70 | 8 |
| | ATOM | 2709 | CB | LEU | B | 68 | 74.066 | -0.198 | 4.001 | 1.00 | 44.25 | 6 |
| | ATOM | 2710 | CG | LEU | B | 68 | 72.989 | -1.184 | 3.489 | 1.00 | 42.50 | 6 |
| 5 | ATOM | 2711 | CD1 | LEU | B | 68 | 72.064 | -1.563 | 4.634 | 1.00 | 40.69 | 6 |
| | ATOM | 2712 | CD2 | LEU | B | 68 | 72.214 | -0.620 | 2.317 | 1.00 | 42.43 | 6 |
| | ATOM | 2713 | N | ALA | B | 69 | 76.513 | -1.866 | 3.793 | 1.00 | 46.99 | 7 |
| | ATOM | 2714 | CA | ALA | B | 69 | 77.238 | -3.024 | 3.259 | 1.00 | 47.49 | 6 |
| 10 | ATOM | 2715 | C | ALA | B | 69 | 77.930 | -3.829 | 4.337 | 1.00 | 46.64 | 6 |
| | ATOM | 2716 | O | ALA | B | 69 | 77.913 | -5.072 | 4.256 | 1.00 | 48.02 | 8 |
| | ATOM | 2717 | CB | ALA | B | 69 | 78.258 | -2.532 | 2.235 | 1.00 | 48.47 | 6 |
| | ATOM | 2718 | N | ARG | B | 70 | 78.475 | -3.201 | 5.370 | 1.00 | 45.74 | 7 |
| | ATOM | 2719 | CA | ARG | B | 70 | 79.158 | -3.961 | 6.411 | 1.00 | 44.24 | 6 |
| 15 | ATOM | 2720 | C | ARG | B | 70 | 78.246 | -4.487 | 7.495 | 1.00 | 44.00 | 6 |
| | ATOM | 2721 | O | ARG | B | 70 | 78.700 | -5.308 | 8.281 | 1.00 | 41.15 | 8 |
| | ATOM | 2722 | CB | ARG | B | 70 | 80.247 | -3.071 | 7.038 | 1.00 | 46.62 | 6 |
| | ATOM | 2723 | N | TYR | B | 71 | 76.966 | -4.108 | 7.573 | 1.00 | 41.84 | 7 |
| | ATOM | 2724 | CA | TYR | B | 71 | 76.076 | -4.624 | 8.609 | 1.00 | 39.35 | 6 |
| 20 | ATOM | 2725 | C | TYR | B | 71 | 75.935 | -6.141 | 8.508 | 1.00 | 37.54 | 6 |
| | ATOM | 2726 | O | TYR | B | 71 | 75.788 | -6.673 | 7.410 | 1.00 | 37.39 | 8 |
| | ATOM | 2727 | CB | TYR | B | 71 | 74.712 | -3.919 | 8.487 | 1.00 | 38.73 | 6 |
| | ATOM | 2728 | CG | TYR | B | 71 | 73.927 | -4.054 | 9.778 | 1.00 | 36.95 | 6 |
| | ATOM | 2729 | CD1 | TYR | B | 71 | 74.099 | -3.155 | 10.806 | 1.00 | 34.97 | 6 |
| 25 | ATOM | 2730 | CD2 | TYR | B | 71 | 72.993 | -5.079 | 9.946 | 1.00 | 35.71 | 6 |
| | ATOM | 2731 | CE1 | TYR | B | 71 | 73.405 | -3.260 | 12.004 | 1.00 | 35.01 | 6 |
| | ATOM | 2732 | CE2 | TYR | B | 71 | 72.287 | -5.192 | 11.109 | 1.00 | 33.37 | 6 |
| | ATOM | 2733 | CZ | TYR | B | 71 | 72.462 | -4.292 | 12.119 | 1.00 | 34.69 | 6 |
| | ATOM | 2734 | OH | TYR | B | 71 | 71.765 | -4.407 | 13.290 | 1.00 | 34.77 | 8 |
| 30 | ATOM | 2735 | N | PRO | B | 72 | 75.985 | -6.835 | 9.625 | 1.00 | 37.73 | 7 |
| | ATOM | 2736 | CA | PRO | B | 72 | 76.030 | -8.293 | 9.644 | 1.00 | 40.09 | 6 |
| | ATOM | 2737 | C | PRO | B | 72 | 74.756 | -8.966 | 9.194 | 1.00 | 42.74 | 6 |
| | ATOM | 2738 | O | PRO | B | 72 | 73.697 | -8.753 | 9.783 | 1.00 | 42.94 | 8 |
| | ATOM | 2739 | CB | PRO | B | 72 | 76.369 | -8.681 | 11.080 | 1.00 | 39.27 | 6 |
| 35 | ATOM | 2740 | CG | PRO | B | 72 | 76.366 | -7.442 | 11.876 | 1.00 | 39.73 | 6 |
| | ATOM | 2741 | CD | PRO | B | 72 | 76.222 | -6.266 | 10.967 | 1.00 | 37.89 | 6 |
| | ATOM | 2742 | N | ARG | B | 73 | 74.856 | -9.773 | 8.147 | 1.00 | 42.53 | 7 |
| | ATOM | 2743 | CA | ARG | B | 73 | 73.687 | -10.492 | 7.639 | 1.00 | 43.36 | 6 |
| | ATOM | 2744 | C | ARG | B | 73 | 73.881 | -11.945 | 7.992 | 1.00 | 43.07 | 6 |
| 40 | ATOM | 2745 | O | ARG | B | 73 | 74.875 | -12.526 | 7.534 | 1.00 | 42.68 | 8 |
| | ATOM | 2746 | CB | ARG | B | 73 | 73.524 | -10.225 | 6.143 | 1.00 | 45.53 | 6 |
| | ATOM | 2747 | CG | ARG | B | 73 | 73.306 | -8.700 | 5.962 | 1.00 | 48.13 | 6 |
| | ATOM | 2748 | CD | ARG | B | 73 | 72.868 | -8.393 | 4.559 | 1.00 | 49.65 | 6 |
| | ATOM | 2749 | NE | ARG | B | 73 | 72.537 | -7.021 | 4.268 | 1.00 | 51.16 | 7 |
| 45 | ATOM | 2750 | CZ | ARG | B | 73 | 73.255 | -5.930 | 4.486 | 1.00 | 51.88 | 6 |
| | ATOM | 2751 | NH1 | ARG | B | 73 | 74.449 | -5.968 | 5.071 | 1.00 | 53.24 | 7 |
| | ATOM | 2752 | NH2 | ARG | B | 73 | 72.779 | -4.755 | 4.085 | 1.00 | 51.96 | 7 |
| | ATOM | 2753 | N | THR | B | 74 | 73.054 | -12.505 | 8.869 | 1.00 | 40.78 | 7 |
| | ATOM | 2754 | CA | THR | B | 74 | 73.184 | -13.870 | 9.338 | 1.00 | 38.76 | 6 |
| 50 | ATOM | 2755 | C | THR | B | 74 | 71.806 | -14.564 | 9.373 | 1.00 | 36.02 | 6 |
| | ATOM | 2756 | O | THR | B | 74 | 71.381 | -15.074 | 10.395 | 1.00 | 35.74 | 8 |
| | ATOM | 2757 | CB | THR | B | 74 | 73.825 | -13.949 | 10.726 | 1.00 | 39.81 | 6 |
| | ATOM | 2758 | OG1 | THR | B | 74 | 72.965 | -13.304 | 11.686 | 1.00 | 41.92 | 8 |
| | ATOM | 2759 | CG2 | THR | B | 74 | 75.176 | -13.231 | 10.872 | 1.00 | 39.68 | 6 |
| 55 | ATOM | 2760 | N | LEU | B | 75 | 71.163 | -14.648 | 8.241 | 1.00 | 38.12 | 7 |
| | ATOM | 2761 | CA | LEU | B | 75 | 69.795 | -15.148 | 8.140 | 1.00 | 38.95 | 6 |
| | ATOM | 2762 | C | LEU | B | 75 | 69.657 | -16.574 | 8.644 | 1.00 | 39.45 | 6 |
| | ATOM | 2763 | O | LEU | B | 75 | 68.791 | -16.843 | 9.478 | 1.00 | 37.24 | 8 |
| | ATOM | 2764 | CB | LEU | B | 75 | 69.269 | -15.024 | 6.693 | 1.00 | 41.95 | 6 |
| 60 | ATOM | 2765 | CG | LEU | B | 75 | 67.785 | -15.355 | 6.505 | 1.00 | 42.42 | 6 |
| | ATOM | 2766 | CD1 | LEU | B | 75 | 66.907 | -14.527 | 7.453 | 1.00 | 43.76 | 6 |
| | ATOM | 2767 | CD2 | LEU | B | 75 | 67.332 | -15.146 | 5.070 | 1.00 | 42.41 | 6 |
| | ATOM | 2768 | N | GLN | B | 76 | 70.525 | -17.509 | 8.187 | 1.00 | 39.28 | 7 |
| | ATOM | 2769 | CA | GLN | B | 76 | 70.400 | -18.884 | 8.667 | 1.00 | 39.73 | 6 |
| 65 | ATOM | 2770 | C | GLN | B | 76 | 70.476 | -18.965 | 10.181 | 1.00 | 36.54 | 6 |
| | ATOM | 2771 | O | GLN | B | 76 | 69.671 | -19.700 | 10.759 | 1.00 | 35.73 | 8 |
| | ATOM | 2772 | CB | GLN | B | 76 | 71.477 | -19.872 | 8.150 | 1.00 | 42.75 | 6 |
| | ATOM | 2773 | CG | GLN | B | 76 | 71.375 | -21.209 | 8.897 | 1.00 | 45.19 | 6 |
| | ATOM | 2774 | CD | GLN | B | 76 | 72.464 | -22.227 | 8.683 | 1.00 | 48.00 | 6 |
| 70 | ATOM | 2775 | OE1 | GLN | B | 76 | 72.386 | -23.355 | 9.236 | 1.00 | 51.20 | 8 |
| | ATOM | 2776 | NE2 | GLN | B | 76 | 73.482 | -21.896 | 7.921 | 1.00 | 46.67 | 7 |
| | ATOM | 2777 | N | GLU | B | 77 | 71.442 | -18.317 | 10.808 | 1.00 | 33.90 | 7 |
| | ATOM | 2778 | CA | GLU | B | 77 | 71.585 | -18.356 | 12.259 | 1.00 | 33.25 | 6 |
| | ATOM | 2779 | C | GLU | B | 77 | 70.408 | -17.708 | 13.013 | 1.00 | 32.48 | 6 |
| | ATOM | 2780 | O | GLU | B | 77 | 69.960 | -18.170 | 14.072 | 1.00 | 31.46 | 8 |

-74-

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|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|----|
| | ATOM | 2781 | CB | GLU | B | 77 | 72.885 | -17.636 | 12.627 | 1.00 | 33.79 | 6 |
| | ATOM | 2782 | N | ASP | B | 78 | 69.915 | -16.625 | 12.388 | 1.00 | 32.55 | 7 |
| | ATOM | 2783 | CA | ASP | B | 78 | 68.738 | -15.937 | 12.973 | 1.00 | 30.24 | 6 |
| 5 | ATOM | 2784 | C | ASP | B | 78 | 67.576 | -16.964 | 12.993 | 1.00 | 28.55 | 6 |
| | ATOM | 2785 | O | ASP | B | 78 | 66.981 | -17.174 | 14.032 | 1.00 | 29.32 | 8 |
| | ATOM | 2786 | CB | ASP | B | 78 | 68.337 | -14.697 | 12.209 | 1.00 | 31.08 | 6 |
| | ATOM | 2787 | CG | ASP | B | 78 | 69.331 | -13.551 | 12.195 | 1.00 | 34.64 | 6 |
| | ATOM | 2788 | OD1 | ASP | B | 78 | 70.144 | -13.494 | 13.151 | 1.00 | 37.80 | 8 |
| 10 | ATOM | 2789 | OD2 | ASP | B | 78 | 69.328 | -12.744 | 11.228 | 1.00 | 36.82 | 8 |
| | ATOM | 2790 | N | CYS | B | 79 | 67.355 | -17.543 | 11.825 | 1.00 | 30.19 | 7 |
| | ATOM | 2791 | CA | CYS | B | 79 | 66.231 | -18.500 | 11.625 | 1.00 | 33.57 | 6 |
| | ATOM | 2792 | C | CYS | B | 79 | 66.327 | -19.720 | 12.495 | 1.00 | 35.51 | 6 |
| | ATOM | 2793 | O | CYS | B | 79 | 65.350 | -20.136 | 13.149 | 1.00 | 34.66 | 8 |
| 15 | ATOM | 2794 | CB | CYS | B | 79 | 66.184 | -18.792 | 10.132 | 1.00 | 33.80 | 6 |
| | ATOM | 2795 | SG | CYS | B | 79 | 65.381 | -17.456 | 9.190 | 1.00 | 37.92 | 16 |
| | ATOM | 2796 | N | GLU | B | 80 | 67.543 | -20.281 | 12.707 | 1.00 | 36.68 | 7 |
| | ATOM | 2797 | CA | GLU | B | 80 | 67.692 | -21.347 | 13.691 | 1.00 | 35.97 | 6 |
| | ATOM | 2798 | C | GLU | B | 80 | 67.370 | -20.883 | 15.088 | 1.00 | 33.68 | 6 |
| 20 | ATOM | 2799 | O | GLU | B | 80 | 66.764 | -21.625 | 15.883 | 1.00 | 34.88 | 8 |
| | ATOM | 2800 | CB | GLU | B | 80 | 69.130 | -21.906 | 13.660 | 1.00 | 36.66 | 6 |
| | ATOM | 2801 | N | LYS | B | 81 | 67.668 | -19.638 | 15.520 | 1.00 | 34.02 | 7 |
| | ATOM | 2802 | CA | LYS | B | 81 | 67.277 | -19.253 | 16.875 | 1.00 | 31.36 | 6 |
| | ATOM | 2803 | C | LYS | B | 81 | 65.756 | -19.047 | 17.017 | 1.00 | 30.38 | 6 |
| 25 | ATOM | 2804 | O | LYS | B | 81 | 65.183 | -19.326 | 18.068 | 1.00 | 29.64 | 8 |
| | ATOM | 2805 | CB | LYS | B | 81 | 67.967 | -17.965 | 17.314 | 1.00 | 35.26 | 6 |
| | ATOM | 2806 | CG | LYS | B | 81 | 69.451 | -18.114 | 17.566 | 1.00 | 37.30 | 6 |
| | ATOM | 2807 | CD | LYS | B | 81 | 70.118 | -16.744 | 17.730 | 1.00 | 39.14 | 6 |
| | ATOM | 2808 | CE | LYS | B | 81 | 71.635 | -17.011 | 17.782 | 1.00 | 41.26 | 6 |
| 30 | ATOM | 2809 | NZ | LYS | B | 81 | 72.310 | -15.733 | 18.142 | 1.00 | 43.00 | 7 |
| | ATOM | 2810 | N | LEU | B | 82 | 65.158 | -18.495 | 15.965 | 1.00 | 30.34 | 7 |
| | ATOM | 2811 | CA | LEU | B | 82 | 63.700 | -18.248 | 16.019 | 1.00 | 30.06 | 6 |
| | ATOM | 2812 | C | LEU | B | 82 | 62.914 | -19.540 | 16.028 | 1.00 | 32.53 | 6 |
| | ATOM | 2813 | O | LEU | B | 82 | 61.880 | -19.695 | 16.694 | 1.00 | 32.69 | 8 |
| 35 | ATOM | 2814 | CB | LEU | B | 82 | 63.335 | -17.328 | 14.845 | 1.00 | 30.48 | 6 |
| | ATOM | 2815 | CG | LEU | B | 82 | 63.981 | -15.924 | 14.936 | 1.00 | 28.69 | 6 |
| | ATOM | 2816 | CD1 | LEU | B | 82 | 63.820 | -15.222 | 13.603 | 1.00 | 25.14 | 6 |
| | ATOM | 2817 | CD2 | LEU | B | 82 | 63.412 | -15.105 | 16.103 | 1.00 | 28.77 | 6 |
| | ATOM | 2818 | N | ASN | B | 83 | 63.438 | -20.549 | 15.323 | 1.00 | 33.22 | 7 |
| 40 | ATOM | 2819 | CA | ASN | B | 83 | 62.748 | -21.849 | 15.282 | 1.00 | 36.28 | 6 |
| | ATOM | 2820 | C | ASN | B | 83 | 62.747 | -22.507 | 16.648 | 1.00 | 36.28 | 6 |
| | ATOM | 2821 | O | ASN | B | 83 | 61.735 | -23.043 | 17.139 | 1.00 | 35.49 | 8 |
| | ATOM | 2822 | CB | ASN | B | 83 | 63.419 | -22.656 | 14.181 | 1.00 | 39.05 | 6 |
| | ATOM | 2823 | CG | ASN | B | 83 | 62.717 | -23.983 | 13.943 | 1.00 | 42.41 | 6 |
| 45 | ATOM | 2824 | OD1 | ASN | B | 83 | 63.382 | -25.000 | 14.194 | 1.00 | 45.42 | 8 |
| | ATOM | 2825 | ND2 | ASN | B | 83 | 61.474 | -23.962 | 13.533 | 1.00 | 41.68 | 7 |
| | ATOM | 2826 | N | LYS | B | 84 | 63.820 | -22.351 | 17.437 | 1.00 | 37.37 | 7 |
| | ATOM | 2827 | CA | LYS | B | 84 | 63.850 | -22.927 | 18.780 | 1.00 | 39.89 | 6 |
| | ATOM | 2828 | C | LYS | B | 84 | 62.942 | -22.200 | 19.747 | 1.00 | 40.11 | 6 |
| 50 | ATOM | 2829 | O | LYS | B | 84 | 62.533 | -22.693 | 20.801 | 1.00 | 40.80 | 8 |
| | ATOM | 2830 | CB | LYS | B | 84 | 65.305 | -22.932 | 19.291 | 1.00 | 39.81 | 6 |
| | ATOM | 2831 | N | ARG | B | 85 | 62.590 | -20.942 | 19.425 | 1.00 | 40.09 | 7 |
| | ATOM | 2832 | CA | ARG | B | 85 | 61.718 | -20.125 | 20.235 | 1.00 | 39.63 | 6 |
| | ATOM | 2833 | C | ARG | B | 85 | 60.260 | -20.305 | 19.812 | 1.00 | 40.59 | 6 |
| 55 | ATOM | 2834 | O | ARG | B | 85 | 59.373 | -19.647 | 20.334 | 1.00 | 42.54 | 8 |
| | ATOM | 2835 | CB | ARG | B | 85 | 62.093 | -18.647 | 20.134 | 1.00 | 40.48 | 6 |
| | ATOM | 2836 | CG | ARG | B | 85 | 62.052 | -17.972 | 21.510 | 1.00 | 41.38 | 6 |
| | ATOM | 2837 | CD | ARG | B | 85 | 63.336 | -18.317 | 22.253 | 1.00 | 42.99 | 6 |
| | ATOM | 2838 | NE | ARG | B | 85 | 63.380 | -17.724 | 23.588 | 1.00 | 42.49 | 7 |
| 60 | ATOM | 2839 | CZ | ARG | B | 85 | 64.475 | -17.764 | 24.342 | 1.00 | 43.47 | 6 |
| | ATOM | 2840 | NH1 | ARG | B | 85 | 64.483 | -17.233 | 25.553 | 1.00 | 42.44 | 7 |
| | ATOM | 2841 | NH2 | ARG | B | 85 | 65.570 | -18.361 | 23.872 | 1.00 | 44.83 | 7 |
| | ATOM | 2842 | N | LYS | B | 86 | 60.041 | -21.151 | 18.827 | 1.00 | 39.06 | 7 |
| | ATOM | 2843 | CA | LYS | B | 86 | 58.702 | -21.492 | 18.348 | 1.00 | 38.48 | 6 |
| 65 | ATOM | 2844 | C | LYS | B | 86 | 57.996 | -20.296 | 17.712 | 1.00 | 36.35 | 6 |
| | ATOM | 2845 | O | LYS | B | 86 | 56.785 | -20.127 | 17.808 | 1.00 | 34.81 | 8 |
| | ATOM | 2846 | CB | LYS | B | 86 | 57.903 | -22.087 | 19.511 | 1.00 | 39.68 | 6 |
| | ATOM | 2847 | N | VAL | B | 87 | 58.751 | -19.515 | 16.953 | 1.00 | 33.22 | 7 |
| | ATOM | 2848 | CA | VAL | B | 87 | 58.133 | -18.416 | 16.204 | 1.00 | 29.42 | 6 |
| 70 | ATOM | 2849 | C | VAL | B | 87 | 57.340 | -18.986 | 15.051 | 1.00 | 30.11 | 6 |
| | ATOM | 2850 | O | VAL | B | 87 | 57.704 | -19.959 | 14.359 | 1.00 | 29.33 | 8 |
| | ATOM | 2851 | CB | VAL | B | 87 | 59.267 | -17.508 | 15.732 | 1.00 | 27.19 | 6 |
| | ATOM | 2852 | CG1 | VAL | B | 87 | 58.859 | -16.637 | 14.581 | 1.00 | 28.11 | 6 |
| | ATOM | 2853 | CG2 | VAL | B | 87 | 59.756 | -16.644 | 16.909 | 1.00 | 28.45 | 6 |
| | ATOM | 2854 | N | ASP | B | 88 | 56.179 | -18.408 | 14.740 | 1.00 | 27.32 | 7 |

-75-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| | ATOM | 2855 | CA | ASP | B | 88 | 55.356 | -18.963 | 13.667 | 1.00 | 26.78 | 6 |
| | ATOM | 2856 | C | ASP | B | 88 | 55.780 | -18.589 | 12.285 | 1.00 | 26.80 | 6 |
| | ATOM | 2857 | O | ASP | B | 88 | 55.687 | -19.415 | 11.342 | 1.00 | 26.44 | 8 |
| 5 | ATOM | 2858 | CB | ASP | B | 88 | 53.895 | -18.488 | 13.889 | 1.00 | 29.04 | 6 |
| | ATOM | 2859 | CG | ASP | B | 88 | 53.482 | -18.856 | 15.298 | 1.00 | 30.71 | 6 |
| | ATOM | 2860 | OD1 | ASP | B | 88 | 52.991 | -20.020 | 15.427 | 1.00 | 32.60 | 8 |
| | ATOM | 2861 | OD2 | ASP | B | 88 | 53.717 | -18.147 | 16.323 | 1.00 | 30.59 | 8 |
| | ATOM | 2862 | N | LEU | B | 89 | 56.204 | -17.356 | 12.062 | 1.00 | 23.49 | 7 |
| 10 | ATOM | 2863 | CA | LEU | B | 89 | 56.498 | -16.854 | 10.756 | 1.00 | 23.51 | 6 |
| | ATOM | 2864 | C | LEU | B | 89 | 57.676 | -15.880 | 10.729 | 1.00 | 23.91 | 6 |
| | ATOM | 2865 | O | LEU | B | 89 | 57.609 | -14.975 | 11.552 | 1.00 | 24.58 | 8 |
| | ATOM | 2866 | CB | LEU | B | 89 | 55.236 | -16.101 | 10.292 | 1.00 | 26.12 | 6 |
| | ATOM | 2867 | CG | LEU | B | 89 | 55.179 | -15.845 | 8.823 | 1.00 | 29.47 | 6 |
| 15 | ATOM | 2868 | CD1 | LEU | B | 89 | 53.725 | -15.783 | 8.333 | 1.00 | 31.30 | 6 |
| | ATOM | 2869 | CD2 | LEU | B | 89 | 55.883 | -14.542 | 8.494 | 1.00 | 32.84 | 6 |
| | ATOM | 2870 | N | VAL | B | 90 | 58.629 | -15.971 | 9.842 | 1.00 | 23.43 | 7 |
| | ATOM | 2871 | CA | VAL | B | 90 | 59.716 | -15.006 | 9.714 | 1.00 | 23.35 | 6 |
| | ATOM | 2872 | C | VAL | B | 90 | 59.553 | -14.315 | 8.413 | 1.00 | 24.66 | 6 |
| 20 | ATOM | 2873 | O | VAL | B | 90 | 59.386 | -14.905 | 7.324 | 1.00 | 24.98 | 8 |
| | ATOM | 2874 | CB | VAL | B | 90 | 61.116 | -15.722 | 9.862 | 1.00 | 23.84 | 6 |
| | ATOM | 2875 | CG1 | VAL | B | 90 | 62.212 | -14.701 | 9.640 | 1.00 | 26.41 | 6 |
| | ATOM | 2876 | CG2 | VAL | B | 90 | 61.195 | -16.379 | 11.217 | 1.00 | 23.75 | 6 |
| | ATOM | 2877 | N | PHE | B | 91 | 59.462 | -12.972 | 8.351 | 1.00 | 23.00 | 7 |
| 25 | ATOM | 2878 | CA | PHE | B | 91 | 59.363 | -12.240 | 7.147 | 1.00 | 21.82 | 6 |
| | ATOM | 2879 | C | PHE | B | 91 | 60.754 | -11.693 | 6.787 | 1.00 | 24.30 | 6 |
| | ATOM | 2880 | O | PHE | B | 91 | 61.258 | -10.892 | 7.578 | 1.00 | 25.55 | 8 |
| | ATOM | 2881 | CB | PHE | B | 91 | 58.346 | -11.073 | 7.207 | 1.00 | 20.44 | 6 |
| | ATOM | 2882 | CG | PHE | B | 91 | 58.180 | -10.275 | 5.969 | 1.00 | 22.85 | 6 |
| 30 | ATOM | 2883 | CD1 | PHE | B | 91 | 58.030 | -10.779 | 4.676 | 1.00 | 21.26 | 6 |
| | ATOM | 2884 | CD2 | PHE | B | 91 | 58.164 | -8.848 | 6.101 | 1.00 | 22.68 | 6 |
| | ATOM | 2885 | CE1 | PHE | B | 91 | 57.900 | -9.976 | 3.571 | 1.00 | 22.13 | 6 |
| | ATOM | 2886 | CE2 | PHE | B | 91 | 58.006 | -8.055 | 4.990 | 1.00 | 21.70 | 6 |
| | ATOM | 2887 | CZ | PHE | B | 91 | 57.852 | -8.587 | 3.703 | 1.00 | 23.17 | 6 |
| 35 | ATOM | 2888 | N | ALA | B | 92 | 61.345 | -12.164 | 5.695 | 1.00 | 24.62 | 7 |
| | ATOM | 2889 | CA | ALA | B | 92 | 62.738 | -11.659 | 5.375 | 1.00 | 23.61 | 6 |
| | ATOM | 2890 | C | ALA | B | 92 | 62.815 | -11.216 | 3.975 | 1.00 | 25.99 | 6 |
| | ATOM | 2891 | O | ALA | B | 92 | 63.216 | -12.052 | 3.123 | 1.00 | 27.84 | 8 |
| | ATOM | 2892 | CB | ALA | B | 92 | 63.656 | -12.811 | 5.743 | 1.00 | 25.77 | 6 |
| 40 | ATOM | 2893 | N | PRO | B | 93 | 62.300 | -10.088 | 3.518 | 1.00 | 25.21 | 7 |
| | ATOM | 2894 | CA | PRO | B | 93 | 62.258 | -9.655 | 2.170 | 1.00 | 26.28 | 6 |
| | ATOM | 2895 | C | PRO | B | 93 | 63.583 | -9.189 | 1.617 | 1.00 | 25.56 | 6 |
| | ATOM | 2896 | O | PRO | B | 93 | 64.455 | -8.761 | 2.381 | 1.00 | 27.95 | 8 |
| | ATOM | 2897 | CB | PRO | B | 93 | 61.283 | -8.471 | 2.238 | 1.00 | 26.93 | 6 |
| 45 | ATOM | 2898 | CG | PRO | B | 93 | 61.547 | -7.888 | 3.586 | 1.00 | 26.11 | 6 |
| | ATOM | 2899 | CD | PRO | B | 93 | 61.769 | -9.060 | 4.516 | 1.00 | 24.38 | 6 |
| | ATOM | 2900 | N | SER | B | 94 | 63.668 | -9.114 | 0.292 | 1.00 | 28.86 | 7 |
| | ATOM | 2901 | CA | SER | B | 94 | 64.891 | -8.524 | -0.309 | 1.00 | 30.21 | 6 |
| | ATOM | 2902 | C | SER | B | 94 | 64.735 | -7.010 | -0.305 | 1.00 | 31.63 | 6 |
| 50 | ATOM | 2903 | O | SER | B | 94 | 63.635 | -6.521 | -0.100 | 1.00 | 27.09 | 8 |
| | ATOM | 2904 | CB | SER | B | 94 | 65.138 | -8.951 | -1.719 | 1.00 | 28.52 | 6 |
| | ATOM | 2905 | OG | SER | B | 94 | 64.254 | -8.353 | -2.673 | 1.00 | 29.83 | 8 |
| | ATOM | 2906 | N | VAL | B | 95 | 65.802 | -6.264 | -0.628 | 1.00 | 32.49 | 7 |
| | ATOM | 2907 | CA | VAL | B | 95 | 65.724 | -4.840 | -0.723 | 1.00 | 31.55 | 6 |
| 55 | ATOM | 2908 | C | VAL | B | 95 | 64.919 | -4.487 | -1.938 | 1.00 | 31.75 | 6 |
| | ATOM | 2909 | O | VAL | B | 95 | 64.138 | -3.540 | -1.883 | 1.00 | 31.41 | 8 |
| | ATOM | 2910 | CB | VAL | B | 95 | 67.144 | -4.172 | -0.780 | 1.00 | 32.74 | 6 |
| | ATOM | 2911 | CG1 | VAL | B | 95 | 67.050 | -2.736 | -1.221 | 1.00 | 34.17 | 6 |
| | ATOM | 2912 | CG2 | VAL | B | 95 | 67.813 | -4.258 | 0.570 | 1.00 | 33.43 | 6 |
| 60 | ATOM | 2913 | N | LYS | B | 96 | 65.004 | -5.262 | -3.023 | 1.00 | 31.26 | 7 |
| | ATOM | 2914 | CA | LYS | B | 96 | 64.226 | -5.022 | -4.212 | 1.00 | 31.62 | 6 |
| | ATOM | 2915 | C | LYS | B | 96 | 62.744 | -5.267 | -3.889 | 1.00 | 29.22 | 6 |
| | ATOM | 2916 | O | LYS | B | 96 | 61.905 | -4.611 | -4.487 | 1.00 | 32.48 | 8 |
| | ATOM | 2917 | CB | LYS | B | 96 | 64.685 | -5.913 | -5.380 | 1.00 | 32.35 | 6 |
| 65 | ATOM | 2918 | N | GLU | B | 97 | 62.464 | -6.172 | -2.988 | 1.00 | 30.27 | 7 |
| | ATOM | 2919 | CA | GLU | B | 97 | 61.056 | -6.463 | -2.667 | 1.00 | 31.03 | 6 |
| | ATOM | 2920 | C | GLU | B | 97 | 60.375 | -5.301 | -1.936 | 1.00 | 30.11 | 6 |
| | ATOM | 2921 | O | GLU | B | 97 | 59.235 | -4.950 | -2.211 | 1.00 | 31.04 | 8 |
| | ATOM | 2922 | CB | GLU | B | 97 | 61.000 | -7.749 | -1.850 | 1.00 | 32.49 | 6 |
| 70 | ATOM | 2923 | CG | GLU | B | 97 | 59.570 | -8.220 | -1.623 | 1.00 | 33.54 | 6 |
| | ATOM | 2924 | CD | GLU | B | 97 | 58.875 | -8.792 | -2.844 | 1.00 | 35.26 | 6 |
| | ATOM | 2925 | OE1 | GLU | B | 97 | 59.540 | -9.132 | -3.867 | 1.00 | 34.07 | 8 |
| | ATOM | 2926 | OE2 | GLU | B | 97 | 57.632 | -8.980 | -2.841 | 1.00 | 32.87 | 8 |
| | ATOM | 2927 | N | ILE | B | 98 | 61.084 | -4.723 | -0.999 | 1.00 | 28.92 | 7 |
| | ATOM | 2928 | CA | ILE | B | 98 | 60.582 | -3.564 | -0.235 | 1.00 | 28.98 | 6 |

-76-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 2929 | C | ILE | B | 98 | 60.727 | -2.241 | -0.955 | 1.00 | 30.40 | 6 |
| | ATOM | 2930 | O | ILE | B | 98 | 59.849 | -1.353 | -0.964 | 1.00 | 25.83 | 8 |
| | ATOM | 2931 | CB | ILE | B | 98 | 61.320 | -3.544 | 1.123 | 1.00 | 26.40 | 6 |
| 5 | ATOM | 2932 | CG1 | ILE | B | 98 | 60.992 | -4.753 | 1.985 | 1.00 | 30.78 | 6 |
| | ATOM | 2933 | CG2 | ILE | B | 98 | 60.988 | -2.241 | 1.865 | 1.00 | 26.02 | 6 |
| | ATOM | 2934 | CD1 | ILE | B | 98 | 59.551 | -5.137 | 2.182 | 1.00 | 30.67 | 6 |
| | ATOM | 2935 | N | TYR | B | 99 | 61.889 | -2.036 | -1.638 | 1.00 | 31.00 | 7 |
| | ATOM | 2936 | CA | TYR | B | 99 | 62.170 | -0.808 | -2.356 | 1.00 | 32.52 | 6 |
| 10 | ATOM | 2937 | C | TYR | B | 99 | 62.505 | -1.034 | -3.812 | 1.00 | 34.54 | 6 |
| | ATOM | 2938 | O | TYR | B | 99 | 63.655 | -0.817 | -4.255 | 1.00 | 35.45 | 8 |
| | ATOM | 2939 | CB | TYR | B | 99 | 63.366 | -0.108 | -1.661 | 1.00 | 31.16 | 6 |
| | ATOM | 2940 | CG | TYR | B | 99 | 63.179 | 0.250 | -0.213 | 1.00 | 28.25 | 6 |
| | ATOM | 2941 | CD1 | TYR | B | 99 | 63.952 | -0.243 | 0.825 | 1.00 | 28.01 | 6 |
| 15 | ATOM | 2942 | CD2 | TYR | B | 99 | 62.202 | 1.193 | 0.117 | 1.00 | 28.98 | 6 |
| | ATOM | 2943 | CE1 | TYR | B | 99 | 63.754 | 0.159 | 2.135 | 1.00 | 27.92 | 6 |
| | ATOM | 2944 | CE2 | TYR | B | 99 | 62.006 | 1.609 | 1.427 | 1.00 | 28.86 | 6 |
| | ATOM | 2945 | CZ | TYR | B | 99 | 62.774 | 1.073 | 2.446 | 1.00 | 27.90 | 6 |
| | ATOM | 2946 | OH | TYR | B | 99 | 62.576 | 1.499 | 3.756 | 1.00 | 27.84 | 8 |
| 20 | ATOM | 2947 | N | PRO | B | 100 | 61.555 | -1.416 | -4.630 | 1.00 | 35.55 | 7 |
| | ATOM | 2948 | CA | PRO | B | 100 | 61.774 | -1.742 | -6.033 | 1.00 | 37.21 | 6 |
| | ATOM | 2949 | C | PRO | B | 100 | 62.327 | -0.598 | -6.843 | 1.00 | 38.72 | 6 |
| | ATOM | 2950 | O | PRO | B | 100 | 63.107 | -0.784 | -7.787 | 1.00 | 39.39 | 8 |
| | ATOM | 2951 | CB | PRO | B | 100 | 60.417 | -2.189 | -6.566 | 1.00 | 37.99 | 6 |
| 25 | ATOM | 2952 | CG | PRO | B | 100 | 59.412 | -1.828 | -5.543 | 1.00 | 35.50 | 6 |
| | ATOM | 2953 | CD | PRO | B | 100 | 60.151 | -1.710 | -4.256 | 1.00 | 35.06 | 6 |
| | ATOM | 2954 | N | ASN | B | 101 | 61.921 | 0.620 | -6.487 | 1.00 | 38.14 | 7 |
| | ATOM | 2955 | CA | ASN | B | 101 | 62.391 | 1.803 | -7.192 | 1.00 | 38.05 | 6 |
| | ATOM | 2956 | C | ASN | B | 101 | 63.459 | 2.537 | -6.385 | 1.00 | 36.99 | 6 |
| 30 | ATOM | 2957 | O | ASN | B | 101 | 63.676 | 3.726 | -6.653 | 1.00 | 39.29 | 8 |
| | ATOM | 2958 | CB | ASN | B | 101 | 61.202 | 2.723 | -7.451 | 1.00 | 39.89 | 6 |
| | ATOM | 2959 | CG | ASN | B | 101 | 60.007 | 1.987 | -8.013 | 1.00 | 41.77 | 6 |
| | ATOM | 2960 | OD1 | ASN | B | 101 | 58.930 | 1.884 | -7.425 | 1.00 | 42.16 | 8 |
| | ATOM | 2961 | ND2 | ASN | B | 101 | 60.229 | 1.436 | -9.197 | 1.00 | 42.54 | 7 |
| 35 | ATOM | 2962 | N | GLY | B | 102 | 64.028 | 1.920 | -5.376 | 1.00 | 34.24 | 7 |
| | ATOM | 2963 | CA | GLY | B | 102 | 64.956 | 2.603 | -4.480 | 1.00 | 33.96 | 6 |
| | ATOM | 2964 | C | GLY | B | 102 | 64.329 | 3.353 | -3.324 | 1.00 | 34.73 | 6 |
| | ATOM | 2965 | O | GLY | B | 102 | 63.091 | 3.507 | -3.190 | 1.00 | 33.28 | 8 |
| | ATOM | 2966 | N | THR | B | 103 | 65.153 | 3.914 | -2.430 | 1.00 | 32.52 | 7 |
| 40 | ATOM | 2967 | CA | THR | B | 103 | 64.591 | 4.613 | -1.279 | 1.00 | 32.04 | 6 |
| | ATOM | 2968 | C | THR | B | 103 | 64.351 | 6.098 | -1.472 | 1.00 | 33.64 | 6 |
| | ATOM | 2969 | O | THR | B | 103 | 63.426 | 6.615 | -0.800 | 1.00 | 32.63 | 8 |
| | ATOM | 2970 | CB | THR | B | 103 | 65.544 | 4.405 | -0.100 | 1.00 | 34.27 | 6 |
| | ATOM | 2971 | OG1 | THR | B | 103 | 66.808 | 4.981 | -0.489 | 1.00 | 34.81 | 8 |
| 45 | ATOM | 2972 | CG2 | THR | B | 103 | 65.762 | 2.948 | 0.225 | 1.00 | 34.11 | 6 |
| | ATOM | 2973 | N | GLU | B | 104 | 65.063 | 6.775 | -2.375 | 1.00 | 31.00 | 7 |
| | ATOM | 2974 | CA | GLU | B | 104 | 64.919 | 8.220 | -2.452 | 1.00 | 34.38 | 6 |
| | ATOM | 2975 | C | GLU | B | 104 | 63.553 | 8.693 | -2.915 | 1.00 | 35.05 | 6 |
| | ATOM | 2976 | O | GLU | B | 104 | 63.205 | 9.837 | -2.567 | 1.00 | 36.53 | 8 |
| 50 | ATOM | 2977 | CB | GLU | B | 104 | 66.012 | 8.810 | -3.394 | 1.00 | 37.66 | 6 |
| | ATOM | 2978 | N | THR | B | 105 | 62.883 | 7.955 | -3.798 | 1.00 | 32.50 | 7 |
| | ATOM | 2979 | CA | THR | B | 105 | 61.572 | 8.395 | -4.264 | 1.00 | 33.06 | 6 |
| | ATOM | 2980 | C | THR | B | 105 | 60.409 | 7.607 | -3.633 | 1.00 | 30.67 | 6 |
| | ATOM | 2981 | O | THR | B | 105 | 59.255 | 7.825 | -4.025 | 1.00 | 30.32 | 8 |
| 55 | ATOM | 2982 | CB | THR | B | 105 | 61.469 | 8.256 | -5.780 | 1.00 | 34.96 | 6 |
| | ATOM | 2983 | OG1 | THR | B | 105 | 61.702 | 6.883 | -6.107 | 1.00 | 35.88 | 8 |
| | ATOM | 2984 | CG2 | THR | B | 105 | 62.498 | 9.147 | -6.493 | 1.00 | 37.41 | 6 |
| | ATOM | 2985 | N | HIS | B | 106 | 60.705 | 6.829 | -2.610 | 1.00 | 28.38 | 7 |
| | ATOM | 2986 | CA | HIS | B | 106 | 59.686 | 6.055 | -1.897 | 1.00 | 26.95 | 6 |
| 60 | ATOM | 2987 | C | HIS | B | 106 | 58.943 | 6.945 | -0.916 | 1.00 | 27.21 | 6 |
| | ATOM | 2988 | O | HIS | B | 106 | 59.558 | 7.820 | -0.286 | 1.00 | 25.40 | 8 |
| | ATOM | 2989 | CB | HIS | B | 106 | 60.299 | 4.906 | -1.129 | 1.00 | 26.76 | 6 |
| | ATOM | 2990 | CG | HIS | B | 106 | 59.397 | 3.804 | -0.619 | 1.00 | 26.50 | 6 |
| | ATOM | 2991 | ND1 | HIS | B | 106 | 58.822 | 3.908 | 0.632 | 1.00 | 26.30 | 7 |
| 65 | ATOM | 2992 | CD2 | HIS | B | 106 | 59.017 | 2.642 | -1.214 | 1.00 | 26.99 | 6 |
| | ATOM | 2993 | CE1 | HIS | B | 106 | 58.139 | 2.730 | 0.807 | 1.00 | 26.31 | 6 |
| | ATOM | 2994 | NE2 | HIS | B | 106 | 58.209 | 1.992 | -0.276 | 1.00 | 27.12 | 7 |
| | ATOM | 2995 | N | THR | B | 107 | 57.621 | 6.749 | -0.815 | 1.00 | 24.60 | 7 |
| | ATOM | 2996 | CA | THR | B | 107 | 56.852 | 7.517 | 0.177 | 1.00 | 22.48 | 6 |
| 70 | ATOM | 2997 | C | THR | B | 107 | 57.510 | 7.428 | 1.528 | 1.00 | 23.26 | 6 |
| | ATOM | 2998 | O | THR | B | 107 | 58.100 | 6.378 | 1.812 | 1.00 | 24.71 | 8 |
| | ATOM | 2999 | CB | THR | B | 107 | 55.425 | 6.933 | 0.229 | 1.00 | 22.11 | 6 |
| | ATOM | 3000 | OG1 | THR | B | 107 | 54.846 | 7.149 | -1.052 | 1.00 | 21.94 | 8 |
| | ATOM | 3001 | CG2 | THR | B | 107 | 54.603 | 7.713 | 1.242 | 1.00 | 24.08 | 6 |
| | ATOM | 3002 | N | TYR | B | 108 | 57.441 | 8.470 | 2.356 | 1.00 | 21.20 | 7 |

-77-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 3003 | CA | TYR | B | 108 | 58.037 | 8.298 | 3.677 | 1.00 | 22.80 | 6 |
| | ATOM | 3004 | C | TYR | B | 108 | 57.170 | 8.870 | 4.799 | 1.00 | 23.19 | 6 |
| | ATOM | 3005 | O | TYR | B | 108 | 56.257 | 9.711 | 4.564 | 1.00 | 20.67 | 8 |
| | ATOM | 3006 | CB | TYR | B | 108 | 59.500 | 8.861 | 3.752 | 1.00 | 26.29 | 6 |
| 5 | ATOM | 3007 | CG | TYR | B | 108 | 59.581 | 10.367 | 3.586 | 1.00 | 27.43 | 6 |
| | ATOM | 3008 | CD1 | TYR | B | 108 | 59.350 | 11.243 | 4.641 | 1.00 | 30.64 | 6 |
| | ATOM | 3009 | CD2 | TYR | B | 108 | 59.795 | 10.914 | 2.331 | 1.00 | 31.95 | 6 |
| | ATOM | 3010 | CE1 | TYR | B | 108 | 59.352 | 12.617 | 4.478 | 1.00 | 31.91 | 6 |
| | ATOM | 3011 | CE2 | TYR | B | 108 | 59.821 | 12.272 | 2.159 | 1.00 | 34.14 | 6 |
| 10 | ATOM | 3012 | CZ | TYR | B | 108 | 59.609 | 13.130 | 3.235 | 1.00 | 34.42 | 6 |
| | ATOM | 3013 | OH | TYR | B | 108 | 59.634 | 14.497 | 3.014 | 1.00 | 36.77 | 8 |
| | ATOM | 3014 | N | VAL | B | 109 | 57.454 | 8.419 | 6.031 | 1.00 | 21.49 | 7 |
| | ATOM | 3015 | CA | VAL | B | 109 | 56.734 | 8.809 | 7.224 | 1.00 | 21.55 | 6 |
| | ATOM | 3016 | C | VAL | B | 109 | 57.707 | 9.552 | 8.149 | 1.00 | 23.45 | 6 |
| 15 | ATOM | 3017 | O | VAL | B | 109 | 58.712 | 8.918 | 8.447 | 1.00 | 22.21 | 8 |
| | ATOM | 3018 | CB | VAL | B | 109 | 56.125 | 7.624 | 8.009 | 1.00 | 20.74 | 6 |
| | ATOM | 3019 | CG1 | VAL | B | 109 | 55.351 | 8.074 | 9.216 | 1.00 | 22.40 | 6 |
| | ATOM | 3020 | CG2 | VAL | B | 109 | 55.248 | 6.829 | 7.006 | 1.00 | 21.59 | 6 |
| 20 | ATOM | 3021 | N | ASP | B | 110 | 57.376 | 10.750 | 8.596 | 1.00 | 22.01 | 7 |
| | ATOM | 3022 | CA | ASP | B | 110 | 58.343 | 11.465 | 9.478 | 1.00 | 24.43 | 6 |
| | ATOM | 3023 | C | ASP | B | 110 | 57.632 | 11.952 | 10.711 | 1.00 | 23.59 | 6 |
| | ATOM | 3024 | O | ASP | B | 110 | 56.504 | 12.458 | 10.672 | 1.00 | 21.44 | 8 |
| | ATOM | 3025 | CB | ASP | B | 110 | 58.991 | 12.648 | 8.759 | 1.00 | 27.76 | 6 |
| | ATOM | 3026 | CG | ASP | B | 110 | 60.461 | 12.751 | 9.239 | 1.00 | 36.19 | 6 |
| 25 | ATOM | 3027 | OD1 | ASP | B | 110 | 61.056 | 12.013 | 10.077 | 1.00 | 37.59 | 8 |
| | ATOM | 3028 | OD2 | ASP | B | 110 | 61.173 | 13.585 | 8.645 | 1.00 | 39.38 | 8 |
| | ATOM | 3029 | N | VAL | B | 111 | 58.257 | 11.795 | 11.892 | 1.00 | 23.56 | 7 |
| | ATOM | 3030 | CA | VAL | B | 111 | 57.669 | 12.175 | 13.148 | 1.00 | 22.23 | 6 |
| 30 | ATOM | 3031 | C | VAL | B | 111 | 58.397 | 13.444 | 13.636 | 1.00 | 26.13 | 6 |
| | ATOM | 3032 | O | VAL | B | 111 | 59.555 | 13.322 | 13.987 | 1.00 | 27.27 | 8 |
| | ATOM | 3033 | CB | VAL | B | 111 | 57.822 | 11.100 | 14.216 | 1.00 | 23.73 | 6 |
| | ATOM | 3034 | CG1 | VAL | B | 111 | 57.213 | 11.440 | 15.574 | 1.00 | 23.64 | 6 |
| | ATOM | 3035 | CG2 | VAL | B | 111 | 57.143 | 9.759 | 13.858 | 1.00 | 24.27 | 6 |
| 35 | ATOM | 3036 | N | PRO | B | 112 | 57.801 | 14.619 | 13.564 | 1.00 | 24.70 | 7 |
| | ATOM | 3037 | CA | PRO | B | 112 | 58.542 | 15.820 | 13.939 | 1.00 | 24.12 | 6 |
| | ATOM | 3038 | C | PRO | B | 112 | 59.048 | 15.823 | 15.355 | 1.00 | 25.44 | 6 |
| | ATOM | 3039 | O | PRO | B | 112 | 58.457 | 15.302 | 16.281 | 1.00 | 25.94 | 8 |
| | ATOM | 3040 | CB | PRO | B | 112 | 57.517 | 16.950 | 13.719 | 1.00 | 26.49 | 6 |
| 40 | ATOM | 3041 | CG | PRO | B | 112 | 56.471 | 16.411 | 12.776 | 1.00 | 25.85 | 6 |
| | ATOM | 3042 | CD | PRO | B | 112 | 56.449 | 14.912 | 13.005 | 1.00 | 25.31 | 6 |
| | ATOM | 3043 | N | GLY | B | 113 | 60.180 | 16.517 | 15.580 | 1.00 | 27.49 | 7 |
| | ATOM | 3044 | CA | GLY | B | 113 | 60.648 | 16.709 | 16.978 | 1.00 | 27.16 | 6 |
| | ATOM | 3045 | C | GLY | B | 113 | 61.466 | 15.490 | 17.404 | 1.00 | 29.14 | 6 |
| | ATOM | 3046 | O | GLY | B | 113 | 62.690 | 15.588 | 17.383 | 1.00 | 29.51 | 8 |
| 45 | ATOM | 3047 | N | LEU | B | 114 | 60.785 | 14.355 | 17.638 | 1.00 | 27.78 | 7 |
| | ATOM | 3048 | CA | LEU | B | 114 | 61.512 | 13.141 | 18.019 | 1.00 | 28.34 | 6 |
| | ATOM | 3049 | C | LEU | B | 114 | 62.545 | 12.685 | 17.019 | 1.00 | 29.38 | 6 |
| | ATOM | 3050 | O | LEU | B | 114 | 63.611 | 12.122 | 17.362 | 1.00 | 28.08 | 8 |
| 50 | ATOM | 3051 | CB | LEU | B | 114 | 60.493 | 12.006 | 18.279 | 1.00 | 26.74 | 6 |
| | ATOM | 3052 | CG | LEU | B | 114 | 59.539 | 12.250 | 19.424 | 1.00 | 28.28 | 6 |
| | ATOM | 3053 | CD1 | LEU | B | 114 | 58.565 | 11.088 | 19.594 | 1.00 | 26.02 | 6 |
| | ATOM | 3054 | CD2 | LEU | B | 114 | 60.295 | 12.476 | 20.742 | 1.00 | 28.90 | 6 |
| | ATOM | 3055 | N | SER | B | 115 | 62.355 | 12.921 | 15.738 | 1.00 | 28.55 | 7 |
| 55 | ATOM | 3056 | CA | SER | B | 115 | 63.262 | 12.446 | 14.710 | 1.00 | 28.22 | 6 |
| | ATOM | 3057 | C | SER | B | 115 | 64.540 | 13.284 | 14.611 | 1.00 | 30.73 | 6 |
| | ATOM | 3058 | O | SER | B | 115 | 65.515 | 12.778 | 14.048 | 1.00 | 29.82 | 8 |
| | ATOM | 3059 | CB | SER | B | 115 | 62.556 | 12.433 | 13.359 | 1.00 | 28.87 | 6 |
| | ATOM | 3060 | OG | SER | B | 115 | 62.188 | 13.728 | 12.878 | 1.00 | 31.15 | 8 |
| 60 | ATOM | 3061 | N | THR | B | 116 | 64.480 | 14.501 | 15.168 | 1.00 | 30.45 | 7 |
| | ATOM | 3062 | CA | THR | B | 116 | 65.625 | 15.383 | 14.934 | 1.00 | 32.38 | 6 |
| | ATOM | 3063 | C | THR | B | 116 | 66.349 | 15.755 | 16.226 | 1.00 | 34.29 | 6 |
| | ATOM | 3064 | O | THR | B | 116 | 67.346 | 16.447 | 16.085 | 1.00 | 38.91 | 8 |
| | ATOM | 3065 | CB | THR | B | 116 | 65.213 | 16.700 | 14.232 | 1.00 | 32.70 | 6 |
| 65 | ATOM | 3066 | OG1 | THR | B | 116 | 64.062 | 17.200 | 14.921 | 1.00 | 32.18 | 8 |
| | ATOM | 3067 | CG2 | THR | B | 116 | 64.868 | 16.509 | 12.776 | 1.00 | 33.85 | 6 |
| | ATOM | 3068 | N | MET | B | 117 | 65.882 | 15.315 | 17.364 | 1.00 | 34.18 | 7 |
| | ATOM | 3069 | CA | MET | B | 117 | 66.556 | 15.577 | 18.625 | 1.00 | 35.31 | 6 |
| | ATOM | 3070 | C | MET | B | 117 | 67.520 | 14.454 | 18.990 | 1.00 | 37.27 | 6 |
| 70 | ATOM | 3071 | O | MET | B | 117 | 67.419 | 13.329 | 18.506 | 1.00 | 35.45 | 8 |
| | ATOM | 3072 | CB | MET | B | 117 | 65.555 | 15.716 | 19.758 | 1.00 | 36.44 | 6 |
| | ATOM | 3073 | CG | MET | B | 117 | 64.825 | 14.432 | 20.149 | 1.00 | 34.64 | 6 |
| | ATOM | 3074 | SD | MET | B | 117 | 63.385 | 14.720 | 21.138 | 1.00 | 35.68 | 16 |
| | ATOM | 3075 | CE | MET | B | 117 | 64.113 | 15.441 | 22.628 | 1.00 | 35.24 | 6 |
| | ATOM | 3076 | N | LEU | B | 118 | 68.432 | 14.767 | 19.943 | 1.00 | 36.08 | 7 |

-78-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3077 | CA | LEU | B | 118 | 69.384 | 13.776 | 20.444 | 1.00 | 35.32 | 6 |
| | ATOM | 3078 | C | LEU | B | 118 | 70.141 | 13.060 | 19.370 | 1.00 | 36.49 | 6 |
| | ATOM | 3079 | O | LEU | B | 118 | 70.769 | 13.672 | 18.490 | 1.00 | 38.03 | 8 |
| 5 | ATOM | 3080 | CB | LEU | B | 118 | 68.602 | 12.780 | 21.326 | 1.00 | 34.52 | 6 |
| | ATOM | 3081 | CG | LEU | B | 118 | 67.955 | 13.401 | 22.550 | 1.00 | 34.53 | 6 |
| | ATOM | 3082 | CD1 | LEU | B | 118 | 67.125 | 12.422 | 23.336 | 1.00 | 33.90 | 6 |
| | ATOM | 3083 | CD2 | LEU | B | 118 | 69.054 | 13.987 | 23.492 | 1.00 | 36.09 | 6 |
| | ATOM | 3084 | N | GLU | B | 119 | 70.061 | 11.719 | 19.302 | 1.00 | 39.19 | 7 |
| 10 | ATOM | 3085 | CA | GLU | B | 119 | 70.748 | 10.969 | 18.252 | 1.00 | 39.90 | 6 |
| | ATOM | 3086 | C | GLU | B | 119 | 70.345 | 11.391 | 16.861 | 1.00 | 39.96 | 6 |
| | ATOM | 3087 | O | GLU | B | 119 | 71.144 | 11.319 | 15.930 | 1.00 | 39.74 | 8 |
| | ATOM | 3088 | CB | GLU | B | 119 | 70.439 | 9.477 | 18.447 | 1.00 | 42.37 | 6 |
| | ATOM | 3089 | CG | GLU | B | 119 | 71.094 | 8.560 | 17.433 | 1.00 | 46.28 | 6 |
| 15 | ATOM | 3090 | CD | GLU | B | 119 | 70.981 | 7.080 | 17.777 | 1.00 | 47.62 | 6 |
| | ATOM | 3091 | OE1 | GLU | B | 119 | 70.337 | 6.733 | 18.805 | 1.00 | 48.65 | 8 |
| | ATOM | 3092 | OE2 | GLU | B | 119 | 71.561 | 6.302 | 16.970 | 1.00 | 49.17 | 8 |
| | ATOM | 3093 | N | GLY | B | 120 | 69.102 | 11.892 | 16.668 | 1.00 | 38.75 | 7 |
| | ATOM | 3094 | CA | GLY | B | 120 | 68.668 | 12.258 | 15.318 | 1.00 | 39.65 | 6 |
| 20 | ATOM | 3095 | C | GLY | B | 120 | 69.318 | 13.524 | 14.807 | 1.00 | 41.25 | 6 |
| | ATOM | 3096 | O | GLY | B | 120 | 69.425 | 13.755 | 13.602 | 1.00 | 39.83 | 8 |
| | ATOM | 3097 | N | ALA | B | 121 | 69.785 | 14.354 | 15.771 | 1.00 | 42.58 | 7 |
| | ATOM | 3098 | CA | ALA | B | 121 | 70.410 | 15.623 | 15.404 | 1.00 | 44.15 | 6 |
| | ATOM | 3099 | C | ALA | B | 121 | 71.647 | 15.421 | 14.552 | 1.00 | 44.51 | 6 |
| 25 | ATOM | 3100 | O | ALA | B | 121 | 71.836 | 16.162 | 13.587 | 1.00 | 46.30 | 8 |
| | ATOM | 3101 | CB | ALA | B | 121 | 70.755 | 16.396 | 16.671 | 1.00 | 44.12 | 6 |
| | ATOM | 3102 | N | SER | B | 122 | 72.464 | 14.428 | 14.839 | 1.00 | 46.51 | 7 |
| | ATOM | 3103 | CA | SER | B | 122 | 73.663 | 14.179 | 14.040 | 1.00 | 48.95 | 6 |
| | ATOM | 3104 | C | SER | B | 122 | 73.442 | 13.166 | 12.932 | 1.00 | 49.98 | 6 |
| 30 | ATOM | 3105 | O | SER | B | 122 | 74.351 | 12.912 | 12.125 | 1.00 | 49.74 | 8 |
| | ATOM | 3106 | CB | SER | B | 122 | 74.790 | 13.675 | 14.943 | 1.00 | 49.52 | 6 |
| | ATOM | 3107 | OG | SER | B | 122 | 74.248 | 12.758 | 15.879 | 1.00 | 51.88 | 8 |
| | ATOM | 3108 | N | ARG | B | 123 | 72.222 | 12.591 | 12.854 | 1.00 | 48.32 | 7 |
| | ATOM | 3109 | CA | ARG | B | 123 | 71.947 | 11.586 | 11.826 | 1.00 | 46.67 | 6 |
| 35 | ATOM | 3110 | C | ARG | B | 123 | 70.694 | 11.919 | 11.018 | 1.00 | 46.85 | 6 |
| | ATOM | 3111 | O | ARG | B | 123 | 69.644 | 11.274 | 11.155 | 1.00 | 45.46 | 8 |
| | ATOM | 3112 | CB | ARG | B | 123 | 71.789 | 10.202 | 12.467 | 1.00 | 46.37 | 6 |
| | ATOM | 3113 | CG | ARG | B | 123 | 72.838 | 9.776 | 13.470 | 1.00 | 46.42 | 6 |
| | ATOM | 3114 | CD | ARG | B | 123 | 72.773 | 8.316 | 13.871 | 1.00 | 46.50 | 6 |
| 40 | ATOM | 3115 | NE | ARG | B | 123 | 72.926 | 7.465 | 12.686 | 1.00 | 47.12 | 7 |
| | ATOM | 3116 | CZ | ARG | B | 123 | 72.709 | 6.151 | 12.722 | 1.00 | 48.23 | 6 |
| | ATOM | 3117 | NH1 | ARG | B | 123 | 72.343 | 5.594 | 13.870 | 1.00 | 48.08 | 7 |
| | ATOM | 3118 | NH2 | ARG | B | 123 | 72.847 | 5.460 | 11.600 | 1.00 | 48.83 | 7 |
| | ATOM | 3119 | N | PRO | B | 124 | 70.814 | 12.888 | 10.125 | 1.00 | 46.75 | 7 |
| 45 | ATOM | 3120 | CA | PRO | B | 124 | 69.724 | 13.307 | 9.272 | 1.00 | 45.09 | 6 |
| | ATOM | 3121 | C | PRO | B | 124 | 69.159 | 12.130 | 8.501 | 1.00 | 43.72 | 6 |
| | ATOM | 3122 | O | PRO | B | 124 | 69.907 | 11.332 | 7.919 | 1.00 | 42.42 | 8 |
| | ATOM | 3123 | CB | PRO | B | 124 | 70.287 | 14.368 | 8.344 | 1.00 | 46.93 | 6 |
| | ATOM | 3124 | CG | PRO | B | 124 | 71.771 | 14.278 | 8.490 | 1.00 | 47.37 | 6 |
| 50 | ATOM | 3125 | CD | PRO | B | 124 | 72.023 | 13.715 | 9.861 | 1.00 | 46.92 | 6 |
| | ATOM | 3126 | N | GLY | B | 125 | 67.828 | 12.007 | 8.537 | 1.00 | 41.20 | 7 |
| | ATOM | 3127 | CA | GLY | B | 125 | 67.230 | 10.900 | 7.774 | 1.00 | 39.29 | 6 |
| | ATOM | 3128 | C | GLY | B | 125 | 67.135 | 9.577 | 8.510 | 1.00 | 37.20 | 6 |
| | ATOM | 3129 | O | GLY | B | 125 | 66.420 | 8.699 | 7.989 | 1.00 | 36.11 | 8 |
| 55 | ATOM | 3130 | N | HIS | B | 126 | 67.837 | 9.368 | 9.601 | 1.00 | 34.73 | 7 |
| | ATOM | 3131 | CA | HIS | B | 126 | 67.849 | 8.102 | 10.308 | 1.00 | 33.50 | 6 |
| | ATOM | 3132 | C | HIS | B | 126 | 66.493 | 7.708 | 10.877 | 1.00 | 32.20 | 6 |
| | ATOM | 3133 | O | HIS | B | 126 | 65.982 | 6.611 | 10.531 | 1.00 | 31.89 | 8 |
| | ATOM | 3134 | CB | HIS | B | 126 | 68.894 | 8.136 | 11.442 | 1.00 | 32.39 | 6 |
| 60 | ATOM | 3135 | CG | HIS | B | 126 | 68.767 | 6.907 | 12.285 | 1.00 | 30.02 | 6 |
| | ATOM | 3136 | ND1 | HIS | B | 126 | 69.142 | 5.669 | 11.764 | 1.00 | 32.16 | 7 |
| | ATOM | 3137 | CD2 | HIS | B | 126 | 68.315 | 6.679 | 13.524 | 1.00 | 28.99 | 6 |
| | ATOM | 3138 | CE1 | HIS | B | 126 | 68.928 | 4.739 | 12.670 | 1.00 | 30.29 | 6 |
| | ATOM | 3139 | NE2 | HIS | B | 126 | 68.411 | 5.323 | 13.726 | 1.00 | 31.28 | 7 |
| 65 | ATOM | 3140 | N | PHE | B | 127 | 65.874 | 8.567 | 11.680 | 1.00 | 28.23 | 7 |
| | ATOM | 3141 | CA | PHE | B | 127 | 64.599 | 8.199 | 12.287 | 1.00 | 27.72 | 6 |
| | ATOM | 3142 | C | PHE | B | 127 | 63.495 | 8.234 | 11.213 | 1.00 | 26.35 | 6 |
| | ATOM | 3143 | O | PHE | B | 127 | 62.599 | 7.393 | 11.386 | 1.00 | 26.75 | 8 |
| | ATOM | 3144 | CB | PHE | B | 127 | 64.268 | 9.034 | 13.528 | 1.00 | 27.25 | 6 |
| 70 | ATOM | 3145 | CG | PHE | B | 127 | 65.109 | 8.550 | 14.698 | 1.00 | 28.04 | 6 |
| | ATOM | 3146 | CD1 | PHE | B | 127 | 66.034 | 9.472 | 15.239 | 1.00 | 27.72 | 6 |
| | ATOM | 3147 | CD2 | PHE | B | 127 | 65.127 | 7.278 | 15.203 | 1.00 | 26.78 | 6 |
| | ATOM | 3148 | CE1 | PHE | B | 127 | 66.838 | 9.035 | 16.291 | 1.00 | 26.75 | 6 |
| | ATOM | 3149 | CE2 | PHE | B | 127 | 65.919 | 6.858 | 16.231 | 1.00 | 29.31 | 6 |
| | ATOM | 3150 | CZ | PHE | B | 127 | 66.844 | 7.755 | 16.771 | 1.00 | 26.94 | 6 |

-79-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3151 | N | ARG | B | 128 | 63.652 | 9.015 | 10.140 | 1.00 | 26.25 | 7 |
| | ATOM | 3152 | CA | ARG | B | 128 | 62.665 | 8.940 | 9.054 | 1.00 | 26.31 | 6 |
| | ATOM | 3153 | C | ARG | B | 128 | 62.641 | 7.529 | 8.474 | 1.00 | 27.01 | 6 |
| 5 | ATOM | 3154 | O | ARG | B | 128 | 61.607 | 6.896 | 8.176 | 1.00 | 27.70 | 8 |
| | ATOM | 3155 | CB | ARG | B | 128 | 62.995 | 9.950 | 7.986 | 1.00 | 29.81 | 6 |
| | ATOM | 3156 | CG | ARG | B | 128 | 62.174 | 9.865 | 6.694 | 1.00 | 28.97 | 6 |
| | ATOM | 3157 | CD | ARG | B | 128 | 62.614 | 10.959 | 5.713 | 1.00 | 31.50 | 6 |
| | ATOM | 3158 | NE | ARG | B | 128 | 62.199 | 12.249 | 6.307 | 1.00 | 36.12 | 7 |
| 10 | ATOM | 3159 | CZ | ARG | B | 128 | 62.359 | 13.422 | 5.685 | 1.00 | 36.94 | 6 |
| | ATOM | 3160 | NH1 | ARG | B | 128 | 62.917 | 13.437 | 4.474 | 1.00 | 36.92 | 7 |
| | ATOM | 3161 | NH2 | ARG | B | 128 | 61.956 | 14.553 | 6.237 | 1.00 | 36.80 | 7 |
| | ATOM | 3162 | N | GLY | B | 129 | 63.823 | 6.942 | 8.316 | 1.00 | 25.53 | 7 |
| | ATOM | 3163 | CA | GLY | B | 129 | 63.959 | 5.579 | 7.803 | 1.00 | 25.39 | 6 |
| 15 | ATOM | 3164 | C | GLY | B | 129 | 63.296 | 4.587 | 8.744 | 1.00 | 24.86 | 6 |
| | ATOM | 3165 | O | GLY | B | 129 | 62.618 | 3.654 | 8.238 | 1.00 | 24.05 | 8 |
| | ATOM | 3166 | N | VAL | B | 130 | 63.374 | 4.723 | 10.054 | 1.00 | 23.36 | 7 |
| | ATOM | 3167 | CA | VAL | B | 130 | 62.752 | 3.848 | 11.024 | 1.00 | 22.23 | 6 |
| | ATOM | 3168 | C | VAL | B | 130 | 61.208 | 3.977 | 10.944 | 1.00 | 23.73 | 6 |
| 20 | ATOM | 3169 | O | VAL | B | 130 | 60.528 | 2.931 | 10.910 | 1.00 | 21.98 | 8 |
| | ATOM | 3170 | CB | VAL | B | 130 | 63.156 | 4.153 | 12.443 | 1.00 | 24.21 | 6 |
| | ATOM | 3171 | CG1 | VAL | B | 130 | 62.503 | 3.325 | 13.534 | 1.00 | 24.51 | 6 |
| | ATOM | 3172 | CG2 | VAL | B | 130 | 64.713 | 3.953 | 12.537 | 1.00 | 24.12 | 6 |
| | ATOM | 3173 | N | SER | B | 131 | 60.667 | 5.199 | 11.057 | 1.00 | 21.64 | 7 |
| 25 | ATOM | 3174 | CA | SER | B | 131 | 59.218 | 5.336 | 11.014 | 1.00 | 21.18 | 6 |
| | ATOM | 3175 | C | SER | B | 131 | 58.706 | 4.864 | 9.647 | 1.00 | 21.42 | 6 |
| | ATOM | 3176 | O | SER | B | 131 | 57.608 | 4.304 | 9.684 | 1.00 | 22.71 | 8 |
| | ATOM | 3177 | CB | SER | B | 131 | 58.790 | 6.781 | 11.406 | 1.00 | 20.10 | 6 |
| | ATOM | 3178 | OG | SER | B | 131 | 59.534 | 7.744 | 10.678 | 1.00 | 22.33 | 8 |
| 30 | ATOM | 3179 | N | THR | B | 132 | 59.376 | 5.073 | 8.538 | 1.00 | 21.18 | 7 |
| | ATOM | 3180 | CA | THR | B | 132 | 58.883 | 4.600 | 7.250 | 1.00 | 22.97 | 6 |
| | ATOM | 3181 | C | THR | B | 132 | 58.795 | 3.079 | 7.224 | 1.00 | 25.11 | 6 |
| | ATOM | 3182 | O | THR | B | 132 | 57.728 | 2.514 | 6.885 | 1.00 | 19.95 | 8 |
| | ATOM | 3183 | CB | THR | B | 132 | 59.742 | 5.139 | 6.108 | 1.00 | 23.70 | 6 |
| 35 | ATOM | 3184 | OG1 | THR | B | 132 | 59.721 | 6.590 | 6.182 | 1.00 | 21.14 | 8 |
| | ATOM | 3185 | CG2 | THR | B | 132 | 59.214 | 4.628 | 4.749 | 1.00 | 21.10 | 6 |
| | ATOM | 3186 | N | ILE | B | 133 | 59.876 | 2.374 | 7.590 | 1.00 | 23.47 | 7 |
| | ATOM | 3187 | CA | ILE | B | 133 | 59.792 | 0.897 | 7.444 | 1.00 | 22.30 | 6 |
| | ATOM | 3188 | C | ILE | B | 133 | 58.868 | 0.339 | 8.499 | 1.00 | 20.08 | 6 |
| 40 | ATOM | 3189 | O | ILE | B | 133 | 58.186 | -0.702 | 8.247 | 1.00 | 20.82 | 8 |
| | ATOM | 3190 | CB | ILE | B | 133 | 61.163 | 0.202 | 7.503 | 1.00 | 22.40 | 6 |
| | ATOM | 3191 | CG1 | ILE | B | 133 | 61.076 | -1.270 | 7.056 | 1.00 | 22.66 | 6 |
| | ATOM | 3192 | CG2 | ILE | B | 133 | 61.699 | 0.252 | 8.924 | 1.00 | 22.72 | 6 |
| | ATOM | 3193 | CD1 | ILE | B | 133 | 60.726 | -1.465 | 5.594 | 1.00 | 24.76 | 6 |
| 45 | ATOM | 3194 | N | VAL | B | 134 | 58.775 | 0.887 | 9.716 | 1.00 | 19.44 | 7 |
| | ATOM | 3195 | CA | VAL | B | 134 | 57.874 | 0.272 | 10.678 | 1.00 | 19.92 | 6 |
| | ATOM | 3196 | C | VAL | B | 134 | 56.425 | 0.507 | 10.228 | 1.00 | 19.95 | 6 |
| | ATOM | 3197 | O | VAL | B | 134 | 55.596 | -0.408 | 10.340 | 1.00 | 18.76 | 8 |
| | ATOM | 3198 | CB | VAL | B | 134 | 58.087 | 0.785 | 12.093 | 1.00 | 20.66 | 6 |
| 50 | ATOM | 3199 | CG1 | VAL | B | 134 | 57.101 | 0.289 | 13.127 | 1.00 | 21.02 | 6 |
| | ATOM | 3200 | CG2 | VAL | B | 134 | 59.472 | 0.315 | 12.628 | 1.00 | 23.22 | 6 |
| | ATOM | 3201 | N | SER | B | 135 | 56.098 | 1.693 | 9.701 | 1.00 | 21.84 | 7 |
| | ATOM | 3202 | CA | SER | B | 135 | 54.738 | 1.882 | 9.197 | 1.00 | 21.43 | 6 |
| | ATOM | 3203 | C | SER | B | 135 | 54.448 | 0.852 | 8.088 | 1.00 | 20.41 | 6 |
| 55 | ATOM | 3204 | O | SER | B | 135 | 53.335 | 0.320 | 8.054 | 1.00 | 19.83 | 8 |
| | ATOM | 3205 | CB | SER | B | 135 | 54.490 | 3.262 | 8.563 | 1.00 | 25.05 | 6 |
| | ATOM | 3206 | OG | SER | B | 135 | 54.496 | 4.192 | 9.637 | 1.00 | 30.48 | 8 |
| | ATOM | 3207 | N | LYS | B | 136 | 55.430 | 0.706 | 7.189 | 1.00 | 18.76 | 7 |
| | ATOM | 3208 | CA | LYS | B | 136 | 55.189 | -0.267 | 6.067 | 1.00 | 20.34 | 6 |
| 60 | ATOM | 3209 | C | LYS | B | 136 | 54.944 | -1.659 | 6.626 | 1.00 | 19.06 | 6 |
| | ATOM | 3210 | O | LYS | B | 136 | 54.010 | -2.371 | 6.185 | 1.00 | 18.19 | 8 |
| | ATOM | 3211 | CB | LYS | B | 136 | 56.351 | -0.243 | 5.052 | 1.00 | 20.12 | 6 |
| | ATOM | 3212 | CG | LYS | B | 136 | 56.143 | -1.143 | 3.805 | 1.00 | 20.78 | 6 |
| | ATOM | 3213 | CD | LYS | B | 136 | 57.014 | -0.638 | 2.664 | 1.00 | 22.99 | 6 |
| 65 | ATOM | 3214 | CE | LYS | B | 136 | 56.995 | -1.594 | 1.478 | 1.00 | 25.34 | 6 |
| | ATOM | 3215 | NZ | LYS | B | 136 | 57.435 | -0.897 | 0.229 | 1.00 | 25.62 | 7 |
| | ATOM | 3216 | N | LEU | B | 137 | 55.713 | -2.120 | 7.604 | 1.00 | 17.80 | 7 |
| | ATOM | 3217 | CA | LEU | B | 137 | 55.582 | -3.427 | 8.237 | 1.00 | 19.98 | 6 |
| | ATOM | 3218 | C | LEU | B | 137 | 54.275 | -3.552 | 8.976 | 1.00 | 19.20 | 6 |
| 70 | ATOM | 3219 | O | LEU | B | 137 | 53.616 | -4.573 | 8.857 | 1.00 | 18.56 | 8 |
| | ATOM | 3220 | CB | LEU | B | 137 | 56.745 | -3.696 | 9.220 | 1.00 | 19.53 | 6 |
| | ATOM | 3221 | CG | LEU | B | 137 | 58.074 | -4.009 | 8.556 | 1.00 | 22.60 | 6 |
| | ATOM | 3222 | CD1 | LEU | B | 137 | 59.179 | -3.990 | 9.627 | 1.00 | 18.94 | 6 |
| | ATOM | 3223 | CD2 | LEU | B | 137 | 58.043 | -5.360 | 7.886 | 1.00 | 20.42 | 6 |
| | ATOM | 3224 | N | PHE | B | 138 | 53.777 | -2.469 | 9.583 | 1.00 | 16.81 | 7 |

-80-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3225 | CA | PHE | B | 138 | 52.487 | -2.532 | 10.200 | 1.00 | 17.03 | 6 |
| | ATOM | 3226 | C | PHE | B | 138 | 51.342 | -2.677 | 9.163 | 1.00 | 15.57 | 6 |
| | ATOM | 3227 | O | PHE | B | 138 | 50.365 | -3.369 | 9.434 | 1.00 | 17.73 | 8 |
| 5 | ATOM | 3228 | CB | PHE | B | 138 | 52.183 | -1.237 | 10.974 | 1.00 | 17.43 | 6 |
| | ATOM | 3229 | CG | PHE | B | 138 | 52.989 | -1.110 | 12.277 | 1.00 | 18.89 | 6 |
| | ATOM | 3230 | CD1 | PHE | B | 138 | 52.929 | 0.069 | 12.997 | 1.00 | 18.99 | 6 |
| | ATOM | 3231 | CD2 | PHE | B | 138 | 53.729 | -2.164 | 12.784 | 1.00 | 19.88 | 6 |
| | ATOM | 3232 | CE1 | PHE | B | 138 | 53.604 | 0.229 | 14.200 | 1.00 | 18.80 | 6 |
| 10 | ATOM | 3233 | CE2 | PHE | B | 138 | 54.411 | -2.031 | 14.006 | 1.00 | 21.38 | 6 |
| | ATOM | 3234 | CZ | PHE | B | 138 | 54.324 | -0.829 | 14.750 | 1.00 | 19.09 | 6 |
| | ATOM | 3235 | N | ASN | B | 139 | 51.457 | -2.015 | 8.033 | 1.00 | 18.34 | 7 |
| | ATOM | 3236 | CA | ASN | B | 139 | 50.419 | -2.157 | 7.032 | 1.00 | 17.77 | 6 |
| | ATOM | 3237 | C | ASN | B | 139 | 50.464 | -3.511 | 6.357 | 1.00 | 18.27 | 6 |
| 15 | ATOM | 3238 | O | ASN | B | 139 | 49.403 | -4.059 | 5.975 | 1.00 | 20.66 | 8 |
| | ATOM | 3239 | CB | ASN | B | 139 | 50.565 | -1.044 | 5.974 | 1.00 | 19.21 | 6 |
| | ATOM | 3240 | CG | ASN | B | 139 | 50.220 | 0.335 | 6.571 | 1.00 | 23.72 | 6 |
| | ATOM | 3241 | OD1 | ASN | B | 139 | 49.304 | 0.418 | 7.359 | 1.00 | 24.33 | 8 |
| | ATOM | 3242 | ND2 | ASN | B | 139 | 50.901 | 1.344 | 6.090 | 1.00 | 25.57 | 7 |
| 20 | ATOM | 3243 | N | LEU | B | 140 | 51.670 | -4.126 | 6.251 | 1.00 | 17.43 | 7 |
| | ATOM | 3244 | CA | LEU | B | 140 | 51.816 | -5.435 | 5.643 | 1.00 | 19.77 | 6 |
| | ATOM | 3245 | C | LEU | B | 140 | 51.392 | -6.531 | 6.585 | 1.00 | 21.88 | 6 |
| | ATOM | 3246 | O | LEU | B | 140 | 50.667 | -7.465 | 6.154 | 1.00 | 22.03 | 8 |
| | ATOM | 3247 | CB | LEU | B | 140 | 53.291 | -5.684 | 5.198 | 1.00 | 18.61 | 6 |
| 25 | ATOM | 3248 | CG | LEU | B | 140 | 53.850 | -4.849 | 4.059 | 1.00 | 20.20 | 6 |
| | ATOM | 3249 | CD1 | LEU | B | 140 | 55.377 | -5.000 | 3.978 | 1.00 | 21.39 | 6 |
| | ATOM | 3250 | CD2 | LEU | B | 140 | 53.219 | -5.272 | 2.744 | 1.00 | 21.81 | 6 |
| | ATOM | 3251 | N | VAL | B | 141 | 51.714 | -6.509 | 7.876 | 1.00 | 19.81 | 7 |
| | ATOM | 3252 | CA | VAL | B | 141 | 51.423 | -7.589 | 8.813 | 1.00 | 19.15 | 6 |
| 30 | ATOM | 3253 | C | VAL | B | 141 | 50.129 | -7.384 | 9.575 | 1.00 | 18.23 | 6 |
| | ATOM | 3254 | O | VAL | B | 141 | 49.508 | -8.383 | 9.942 | 1.00 | 20.17 | 8 |
| | ATOM | 3255 | CB | VAL | B | 141 | 52.613 | -7.729 | 9.811 | 1.00 | 18.50 | 6 |
| | ATOM | 3256 | CG1 | VAL | B | 141 | 52.402 | -8.790 | 10.886 | 1.00 | 19.99 | 6 |
| | ATOM | 3257 | CG2 | VAL | B | 141 | 53.895 | -8.020 | 9.003 | 1.00 | 21.20 | 6 |
| 35 | ATOM | 3258 | N | GLN | B | 142 | 49.697 | -6.125 | 9.766 | 1.00 | 19.03 | 7 |
| | ATOM | 3259 | CA | GLN | B | 142 | 48.456 | -5.803 | 10.496 | 1.00 | 18.67 | 6 |
| | ATOM | 3260 | C | GLN | B | 142 | 48.367 | -6.472 | 11.813 | 1.00 | 18.44 | 6 |
| | ATOM | 3261 | O | GLN | B | 142 | 47.434 | -7.193 | 12.153 | 1.00 | 18.66 | 8 |
| 40 | ATOM | 3262 | CB | GLN | B | 142 | 47.254 | -6.242 | 9.585 | 1.00 | 23.65 | 6 |
| | ATOM | 3263 | CG | GLN | B | 142 | 47.341 | -5.370 | 8.311 | 1.00 | 27.77 | 6 |
| | ATOM | 3264 | CD | GLN | B | 142 | 46.179 | -5.714 | 7.395 | 1.00 | 31.08 | 6 |
| | ATOM | 3265 | OE1 | GLN | B | 142 | 45.039 | -5.391 | 7.745 | 1.00 | 34.74 | 8 |
| | ATOM | 3266 | NE2 | GLN | B | 142 | 46.447 | -6.335 | 6.281 | 1.00 | 33.99 | 7 |
| | ATOM | 3267 | N | PRO | B | 143 | 49.444 | -6.363 | 12.645 | 1.00 | 19.66 | 7 |
| 45 | ATOM | 3268 | CA | PRO | B | 143 | 49.526 | -7.003 | 13.913 | 1.00 | 21.32 | 6 |
| | ATOM | 3269 | C | PRO | B | 143 | 48.579 | -6.373 | 14.939 | 1.00 | 20.88 | 6 |
| | ATOM | 3270 | O | PRO | B | 143 | 48.162 | -5.222 | 14.777 | 1.00 | 23.53 | 8 |
| | ATOM | 3271 | CB | PRO | B | 143 | 50.974 | -6.829 | 14.398 | 1.00 | 19.63 | 6 |
| | ATOM | 3272 | CG | PRO | B | 143 | 51.245 | -5.445 | 13.833 | 1.00 | 20.10 | 6 |
| 50 | ATOM | 3273 | CD | PRO | B | 143 | 50.576 | -5.419 | 12.433 | 1.00 | 20.21 | 6 |
| | ATOM | 3274 | N | ASP | B | 144 | 48.242 | -7.127 | 15.964 | 1.00 | 19.65 | 7 |
| | ATOM | 3275 | CA | ASP | B | 144 | 47.481 | -6.572 | 17.069 | 1.00 | 19.58 | 6 |
| | ATOM | 3276 | C | ASP | B | 144 | 48.443 | -5.798 | 17.998 | 1.00 | 20.96 | 6 |
| | ATOM | 3277 | O | ASP | B | 144 | 48.078 | -4.862 | 18.701 | 1.00 | 21.10 | 8 |
| 55 | ATOM | 3278 | CB | ASP | B | 144 | 46.769 | -7.645 | 17.857 | 1.00 | 21.71 | 6 |
| | ATOM | 3279 | CG | ASP | B | 144 | 45.715 | -8.336 | 16.977 | 1.00 | 29.09 | 6 |
| | ATOM | 3280 | OD1 | ASP | B | 144 | 46.026 | -9.413 | 16.419 | 1.00 | 28.54 | 8 |
| | ATOM | 3281 | OD2 | ASP | B | 144 | 44.670 | -7.652 | 16.763 | 1.00 | 29.74 | 8 |
| | ATOM | 3282 | N | ILE | B | 145 | 49.639 | -6.395 | 18.133 | 1.00 | 19.56 | 7 |
| 60 | ATOM | 3283 | CA | ILE | B | 145 | 50.662 | -5.948 | 19.117 | 1.00 | 20.94 | 6 |
| | ATOM | 3284 | C | ILE | B | 145 | 52.010 | -5.887 | 18.446 | 1.00 | 19.85 | 6 |
| | ATOM | 3285 | O | ILE | B | 145 | 52.279 | -6.676 | 17.481 | 1.00 | 19.52 | 8 |
| | ATOM | 3286 | CB | ILE | B | 145 | 50.680 | -6.958 | 20.269 | 1.00 | 21.71 | 6 |
| | ATOM | 3287 | CG1 | ILE | B | 145 | 49.386 | -6.954 | 21.122 | 1.00 | 24.70 | 6 |
| 65 | ATOM | 3288 | CG2 | ILE | B | 145 | 51.900 | -6.729 | 21.173 | 1.00 | 26.93 | 6 |
| | ATOM | 3289 | CD1 | ILE | B | 145 | 49.072 | -8.328 | 21.695 | 1.00 | 28.80 | 6 |
| | ATOM | 3290 | N | ALA | B | 146 | 52.910 | -4.978 | 18.807 | 1.00 | 20.13 | 7 |
| | ATOM | 3291 | CA | ALA | B | 146 | 54.247 | -4.939 | 18.221 | 1.00 | 20.86 | 6 |
| | ATOM | 3292 | C | ALA | B | 146 | 55.243 | -4.703 | 19.396 | 1.00 | 23.49 | 6 |
| 70 | ATOM | 3293 | O | ALA | B | 146 | 54.897 | -3.879 | 20.234 | 1.00 | 21.46 | 8 |
| | ATOM | 3294 | CB | ALA | B | 146 | 54.442 | -3.869 | 17.206 | 1.00 | 21.57 | 6 |
| | ATOM | 3295 | N | CYS | B | 147 | 56.282 | -5.520 | 19.470 | 1.00 | 21.24 | 7 |
| | ATOM | 3296 | CA | CYS | B | 147 | 57.227 | -5.418 | 20.634 | 1.00 | 21.57 | 6 |
| | ATOM | 3297 | C | CYS | B | 147 | 58.514 | -4.835 | 20.232 | 1.00 | 19.68 | 6 |
| | ATOM | 3298 | O | CYS | B | 147 | 59.148 | -5.086 | 19.189 | 1.00 | 23.55 | 8 |

-81-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 3299 | CB | CYS | B | 147 | 57.487 | -6.803 | 21.192 | 1.00 | 25.97 | 6 |
| | ATOM | 3300 | SG | CYS | B | 147 | 56.049 | -7.649 | 21.811 | 1.00 | 30.41 | 16 |
| | ATOM | 3301 | N | PHE | B | 148 | 59.070 | -3.904 | 21.116 | 1.00 | 21.36 | 7 |
| | ATOM | 3302 | CA | PHE | B | 148 | 60.268 | -3.195 | 20.823 | 1.00 | 19.98 | 6 |
| 5 | ATOM | 3303 | C | PHE | B | 148 | 61.134 | -3.123 | 22.146 | 1.00 | 19.23 | 6 |
| | ATOM | 3304 | O | PHE | B | 148 | 60.479 | -3.140 | 23.148 | 1.00 | 23.93 | 8 |
| | ATOM | 3305 | CB | PHE | B | 148 | 60.072 | -1.760 | 20.374 | 1.00 | 22.31 | 6 |
| | ATOM | 3306 | CG | PHE | B | 148 | 59.349 | -1.636 | 19.056 | 1.00 | 21.62 | 6 |
| 10 | ATOM | 3307 | CD1 | PHE | B | 148 | 57.968 | -1.677 | 19.110 | 1.00 | 22.35 | 6 |
| | ATOM | 3308 | CD2 | PHE | B | 148 | 60.045 | -1.548 | 17.891 | 1.00 | 24.41 | 6 |
| | ATOM | 3309 | CE1 | PHE | B | 148 | 57.226 | -1.664 | 17.918 | 1.00 | 21.17 | 6 |
| | ATOM | 3310 | CE2 | PHE | B | 148 | 59.307 | -1.425 | 16.674 | 1.00 | 23.20 | 6 |
| | ATOM | 3311 | CZ | PHE | B | 148 | 57.930 | -1.509 | 16.754 | 1.00 | 19.10 | 6 |
| 15 | ATOM | 3312 | N | GLY | B | 149 | 62.415 | -3.168 | 22.002 | 1.00 | 22.90 | 7 |
| | ATOM | 3313 | CA | GLY | B | 149 | 63.243 | -3.177 | 23.235 | 1.00 | 24.26 | 6 |
| | ATOM | 3314 | C | GLY | B | 149 | 63.315 | -1.783 | 23.884 | 1.00 | 26.58 | 6 |
| | ATOM | 3315 | O | GLY | B | 149 | 63.397 | -0.779 | 23.199 | 1.00 | 27.16 | 8 |
| | ATOM | 3316 | N | GLU | B | 150 | 63.380 | -1.759 | 25.212 | 1.00 | 27.01 | 7 |
| 20 | ATOM | 3317 | CA | GLU | B | 150 | 63.530 | -0.425 | 25.870 | 1.00 | 29.68 | 6 |
| | ATOM | 3318 | C | GLU | B | 150 | 64.894 | 0.200 | 25.737 | 1.00 | 31.07 | 6 |
| | ATOM | 3319 | O | GLU | B | 150 | 65.020 | 1.425 | 25.978 | 1.00 | 30.50 | 8 |
| | ATOM | 3320 | CB | GLU | B | 150 | 63.214 | -0.532 | 27.368 | 1.00 | 31.68 | 6 |
| | ATOM | 3321 | CG | GLU | B | 150 | 61.747 | -0.632 | 27.660 | 1.00 | 34.09 | 6 |
| 25 | ATOM | 3322 | CD | GLU | B | 150 | 61.359 | -0.743 | 29.111 | 1.00 | 37.99 | 6 |
| | ATOM | 3323 | OE1 | GLU | B | 150 | 62.205 | -0.936 | 30.001 | 1.00 | 38.43 | 8 |
| | ATOM | 3324 | OE2 | GLU | B | 150 | 60.143 | -0.643 | 29.350 | 1.00 | 40.17 | 8 |
| | ATOM | 3325 | N | LYS | B | 151 | 65.951 | -0.544 | 25.401 | 1.00 | 29.23 | 7 |
| | ATOM | 3326 | CA | LYS | B | 151 | 67.258 | 0.093 | 25.292 | 1.00 | 31.41 | 6 |
| 30 | ATOM | 3327 | C | LYS | B | 151 | 67.273 | 1.220 | 24.300 | 1.00 | 31.27 | 6 |
| | ATOM | 3328 | O | LYS | B | 151 | 67.936 | 2.260 | 24.433 | 1.00 | 27.21 | 8 |
| | ATOM | 3329 | CB | LYS | B | 151 | 68.320 | -0.926 | 24.878 | 1.00 | 34.10 | 6 |
| | ATOM | 3330 | CG | LYS | B | 151 | 69.755 | -0.397 | 24.923 | 1.00 | 37.66 | 6 |
| | ATOM | 3331 | CD | LYS | B | 151 | 70.640 | -1.476 | 24.317 | 1.00 | 41.05 | 6 |
| 35 | ATOM | 3332 | CE | LYS | B | 151 | 72.080 | -1.431 | 24.765 | 1.00 | 43.98 | 6 |
| | ATOM | 3333 | NZ | LYS | B | 151 | 72.893 | -0.452 | 23.975 | 1.00 | 44.59 | 7 |
| | ATOM | 3334 | N | ASP | B | 152 | 66.506 | 1.027 | 23.164 | 1.00 | 28.39 | 7 |
| | ATOM | 3335 | CA | ASP | B | 152 | 66.518 | 2.032 | 22.110 | 1.00 | 28.38 | 6 |
| | ATOM | 3336 | C | ASP | B | 152 | 65.332 | 2.937 | 22.374 | 1.00 | 28.23 | 6 |
| 40 | ATOM | 3337 | O | ASP | B | 152 | 64.210 | 2.803 | 21.783 | 1.00 | 26.26 | 8 |
| | ATOM | 3338 | CB | ASP | B | 152 | 66.440 | 1.375 | 20.725 | 1.00 | 28.61 | 6 |
| | ATOM | 3339 | N | PHE | B | 153 | 65.516 | 3.702 | 23.467 | 1.00 | 25.07 | 7 |
| | ATOM | 3340 | CA | PHE | B | 153 | 64.373 | 4.471 | 23.974 | 1.00 | 26.53 | 6 |
| | ATOM | 3341 | C | PHE | B | 153 | 63.892 | 5.520 | 22.974 | 1.00 | 21.61 | 6 |
| 45 | ATOM | 3342 | O | PHE | B | 153 | 62.708 | 5.839 | 23.024 | 1.00 | 24.77 | 8 |
| | ATOM | 3343 | CB | PHE | B | 153 | 64.730 | 5.118 | 25.330 | 1.00 | 26.51 | 6 |
| | ATOM | 3344 | CG | PHE | B | 153 | 65.779 | 6.167 | 25.190 | 1.00 | 29.71 | 6 |
| | ATOM | 3345 | CD1 | PHE | B | 153 | 65.443 | 7.493 | 24.943 | 1.00 | 29.96 | 6 |
| | ATOM | 3346 | CD2 | PHE | B | 153 | 67.132 | 5.855 | 25.398 | 1.00 | 29.77 | 6 |
| 50 | ATOM | 3347 | CE1 | PHE | B | 153 | 66.423 | 8.454 | 24.846 | 1.00 | 31.18 | 6 |
| | ATOM | 3348 | CE2 | PHE | B | 153 | 68.099 | 6.820 | 25.256 | 1.00 | 28.84 | 6 |
| | ATOM | 3349 | CZ | PHE | B | 153 | 67.763 | 8.135 | 24.997 | 1.00 | 31.32 | 6 |
| | ATOM | 3350 | N | GLN | B | 154 | 64.740 | 6.002 | 22.113 | 1.00 | 23.01 | 7 |
| | ATOM | 3351 | CA | GLN | B | 154 | 64.352 | 7.012 | 21.149 | 1.00 | 24.58 | 6 |
| 55 | ATOM | 3352 | C | GLN | B | 154 | 63.443 | 6.353 | 20.075 | 1.00 | 24.87 | 6 |
| | ATOM | 3353 | O | GLN | B | 154 | 62.466 | 6.997 | 19.707 | 1.00 | 23.87 | 8 |
| | ATOM | 3354 | CB | GLN | B | 154 | 65.558 | 7.664 | 20.502 | 1.00 | 26.01 | 6 |
| | ATOM | 3355 | CG | GLN | B | 154 | 65.117 | 8.877 | 19.710 | 1.00 | 28.34 | 6 |
| | ATOM | 3356 | CD | GLN | B | 154 | 66.171 | 9.934 | 19.456 | 1.00 | 30.51 | 6 |
| 60 | ATOM | 3357 | OE1 | GLN | B | 154 | 67.342 | 9.742 | 19.766 | 1.00 | 32.27 | 8 |
| | ATOM | 3358 | NE2 | GLN | B | 154 | 65.742 | 11.030 | 18.839 | 1.00 | 28.70 | 7 |
| | ATOM | 3359 | N | GLN | B | 155 | 63.841 | 5.183 | 19.619 | 1.00 | 24.42 | 7 |
| | ATOM | 3360 | CA | GLN | B | 155 | 62.944 | 4.439 | 18.714 | 1.00 | 24.63 | 6 |
| | ATOM | 3361 | C | GLN | B | 155 | 61.612 | 4.204 | 19.382 | 1.00 | 22.70 | 6 |
| 65 | ATOM | 3362 | O | GLN | B | 155 | 60.577 | 4.285 | 18.652 | 1.00 | 24.30 | 8 |
| | ATOM | 3363 | CB | GLN | B | 155 | 63.549 | 3.094 | 18.268 | 1.00 | 25.06 | 6 |
| | ATOM | 3364 | CG | GLN | B | 155 | 64.450 | 3.209 | 17.029 | 1.00 | 29.61 | 6 |
| | ATOM | 3365 | CD | GLN | B | 155 | 64.506 | 1.856 | 16.285 | 1.00 | 32.67 | 6 |
| | ATOM | 3366 | OE1 | GLN | B | 155 | 65.360 | 1.610 | 15.440 | 1.00 | 37.92 | 8 |
| 70 | ATOM | 3367 | NE2 | GLN | B | 155 | 63.610 | 0.953 | 16.599 | 1.00 | 28.61 | 7 |
| | ATOM | 3368 | N | LEU | B | 156 | 61.522 | 3.748 | 20.602 | 1.00 | 20.20 | 7 |
| | ATOM | 3369 | CA | LEU | B | 156 | 60.288 | 3.409 | 21.273 | 1.00 | 22.81 | 6 |
| | ATOM | 3370 | C | LEU | B | 156 | 59.381 | 4.671 | 21.280 | 1.00 | 25.01 | 6 |
| | ATOM | 3371 | O | LEU | B | 156 | 58.192 | 4.596 | 20.961 | 1.00 | 22.03 | 8 |
| | ATOM | 3372 | CB | LEU | B | 156 | 60.549 | 2.887 | 22.651 | 1.00 | 23.28 | 6 |

-82-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 3373 | CG | LEU | B | 156 | 59.393 | 2.429 | 23.497 | 1.00 | 22.55 | 6 |
| | ATOM | 3374 | CD1 | LEU | B | 156 | 58.484 | 1.403 | 22.784 | 1.00 | 24.60 | 6 |
| | ATOM | 3375 | CD2 | LEU | B | 156 | 59.895 | 1.814 | 24.812 | 1.00 | 24.72 | 6 |
| 5 | ATOM | 3376 | N | ALA | B | 157 | 59.971 | 5.799 | 21.745 | 1.00 | 21.98 | 7 |
| | ATOM | 3377 | CA | ALA | B | 157 | 59.149 | 7.006 | 21.699 | 1.00 | 23.16 | 6 |
| | ATOM | 3378 | C | ALA | B | 157 | 58.684 | 7.366 | 20.300 | 1.00 | 21.84 | 6 |
| | ATOM | 3379 | O | ALA | B | 157 | 57.504 | 7.836 | 20.225 | 1.00 | 22.95 | 8 |
| | ATOM | 3380 | CB | ALA | B | 157 | 59.953 | 8.235 | 22.216 | 1.00 | 21.48 | 6 |
| 10 | ATOM | 3381 | N | LEU | B | 158 | 59.510 | 7.286 | 19.278 | 1.00 | 20.55 | 7 |
| | ATOM | 3382 | CA | LEU | B | 158 | 59.209 | 7.601 | 17.902 | 1.00 | 24.17 | 6 |
| | ATOM | 3383 | C | LEU | B | 158 | 58.018 | 6.737 | 17.408 | 1.00 | 24.35 | 6 |
| | ATOM | 3384 | O | LEU | B | 158 | 57.063 | 7.345 | 16.896 | 1.00 | 21.76 | 8 |
| | ATOM | 3385 | CB | LEU | B | 158 | 60.387 | 7.347 | 16.959 | 1.00 | 23.67 | 6 |
| 15 | ATOM | 3386 | CG | LEU | B | 158 | 60.332 | 7.840 | 15.511 | 1.00 | 25.33 | 6 |
| | ATOM | 3387 | CD1 | LEU | B | 158 | 60.910 | 9.254 | 15.385 | 1.00 | 25.04 | 6 |
| | ATOM | 3388 | CD2 | LEU | B | 158 | 61.078 | 6.855 | 14.633 | 1.00 | 24.59 | 6 |
| | ATOM | 3389 | N | ILE | B | 159 | 58.085 | 5.451 | 17.683 | 1.00 | 21.94 | 7 |
| | ATOM | 3390 | CA | ILE | B | 159 | 56.938 | 4.578 | 17.235 | 1.00 | 22.18 | 6 |
| 20 | ATOM | 3391 | C | ILE | B | 159 | 55.685 | 4.727 | 18.032 | 1.00 | 24.01 | 6 |
| | ATOM | 3392 | O | ILE | B | 159 | 54.587 | 4.804 | 17.414 | 1.00 | 21.79 | 8 |
| | ATOM | 3393 | CB | ILE | B | 159 | 57.436 | 3.108 | 17.263 | 1.00 | 21.63 | 6 |
| | ATOM | 3394 | CG1 | ILE | B | 159 | 58.615 | 3.036 | 16.314 | 1.00 | 21.10 | 6 |
| | ATOM | 3395 | CG2 | ILE | B | 159 | 56.305 | 2.118 | 16.906 | 1.00 | 21.29 | 6 |
| 25 | ATOM | 3396 | CD1 | ILE | B | 159 | 58.290 | 3.361 | 14.848 | 1.00 | 27.17 | 6 |
| | ATOM | 3397 | N | ARG | B | 160 | 55.764 | 5.016 | 19.357 | 1.00 | 21.20 | 7 |
| | ATOM | 3398 | CA | ARG | B | 160 | 54.563 | 5.304 | 20.113 | 1.00 | 23.22 | 6 |
| | ATOM | 3399 | C | ARG | B | 160 | 53.911 | 6.620 | 19.579 | 1.00 | 20.84 | 6 |
| | ATOM | 3400 | O | ARG | B | 160 | 52.688 | 6.604 | 19.482 | 1.00 | 22.99 | 8 |
| 30 | ATOM | 3401 | CB | ARG | B | 160 | 54.786 | 5.438 | 21.627 | 1.00 | 22.64 | 6 |
| | ATOM | 3402 | CG | ARG | B | 160 | 54.975 | 4.035 | 22.266 | 1.00 | 25.40 | 6 |
| | ATOM | 3403 | CD | ARG | B | 160 | 55.364 | 4.303 | 23.720 | 0.50 | 28.99 | 6 |
| | ATOM | 3404 | NE | ARG | B | 160 | 55.627 | 3.143 | 24.540 | 0.50 | 32.14 | 7 |
| | ATOM | 3405 | CZ | ARG | B | 160 | 54.843 | 2.116 | 24.819 | 0.50 | 32.06 | 6 |
| 35 | ATOM | 3406 | NH1 | ARG | B | 160 | 53.609 | 1.993 | 24.361 | 0.50 | 31.32 | 7 |
| | ATOM | 3407 | NH2 | ARG | B | 160 | 55.288 | 1.143 | 25.624 | 0.50 | 32.40 | 7 |
| | ATOM | 3408 | N | LYS | B | 161 | 54.699 | 7.617 | 19.257 | 1.00 | 20.06 | 7 |
| | ATOM | 3409 | CA | LYS | B | 161 | 54.121 | 8.866 | 18.707 | 1.00 | 19.89 | 6 |
| | ATOM | 3410 | C | LYS | B | 161 | 53.502 | 8.570 | 17.331 | 1.00 | 20.88 | 6 |
| 40 | ATOM | 3411 | O | LYS | B | 161 | 52.418 | 9.085 | 17.017 | 1.00 | 20.38 | 8 |
| | ATOM | 3412 | CB | LYS | B | 161 | 55.172 | 9.998 | 18.633 | 1.00 | 21.42 | 6 |
| | ATOM | 3413 | CG | LYS | B | 161 | 54.474 | 11.290 | 18.133 | 1.00 | 23.56 | 6 |
| | ATOM | 3414 | CD | LYS | B | 161 | 55.345 | 12.508 | 18.131 | 1.00 | 27.88 | 6 |
| | ATOM | 3415 | CE | LYS | B | 161 | 54.736 | 13.692 | 17.336 | 1.00 | 31.75 | 6 |
| 45 | ATOM | 3416 | NZ | LYS | B | 161 | 53.349 | 13.890 | 17.879 | 1.00 | 29.32 | 7 |
| | ATOM | 3417 | N | MET | B | 162 | 54.244 | 7.875 | 16.465 | 1.00 | 19.25 | 7 |
| | ATOM | 3418 | CA | MET | B | 162 | 53.744 | 7.586 | 15.106 | 1.00 | 20.25 | 6 |
| | ATOM | 3419 | C | MET | B | 162 | 52.443 | 6.849 | 15.190 | 1.00 | 20.77 | 6 |
| | ATOM | 3420 | O | MET | B | 162 | 51.432 | 7.100 | 14.451 | 1.00 | 20.50 | 8 |
| 50 | ATOM | 3421 | CB | MET | B | 162 | 54.864 | 6.798 | 14.378 | 1.00 | 20.27 | 6 |
| | ATOM | 3422 | CG | MET | B | 162 | 54.438 | 6.504 | 12.918 | 1.00 | 20.30 | 6 |
| | ATOM | 3423 | SD | MET | B | 162 | 55.575 | 5.209 | 12.231 | 1.00 | 23.99 | 16 |
| | ATOM | 3424 | CE | MET | B | 162 | 54.976 | 3.754 | 13.066 | 1.00 | 22.75 | 6 |
| | ATOM | 3425 | N | VAL | B | 163 | 52.331 | 5.858 | 16.110 | 1.00 | 19.38 | 7 |
| 55 | ATOM | 3426 | CA | VAL | B | 163 | 51.106 | 5.095 | 16.243 | 1.00 | 20.12 | 6 |
| | ATOM | 3427 | C | VAL | B | 163 | 49.926 | 5.955 | 16.693 | 1.00 | 22.03 | 6 |
| | ATOM | 3428 | O | VAL | B | 163 | 48.820 | 5.841 | 16.163 | 1.00 | 19.78 | 8 |
| | ATOM | 3429 | CB | VAL | B | 163 | 51.310 | 3.926 | 17.212 | 1.00 | 19.66 | 6 |
| | ATOM | 3430 | CG1 | VAL | B | 163 | 50.044 | 3.269 | 17.672 | 1.00 | 20.89 | 6 |
| 60 | ATOM | 3431 | CG2 | VAL | B | 163 | 52.253 | 2.958 | 16.455 | 1.00 | 20.73 | 6 |
| | ATOM | 3432 | N | ALA | B | 164 | 50.127 | 6.771 | 17.688 | 1.00 | 20.47 | 7 |
| | ATOM | 3433 | CA | ALA | B | 164 | 49.065 | 7.634 | 18.189 | 1.00 | 21.69 | 6 |
| | ATOM | 3434 | C | ALA | B | 164 | 48.642 | 8.624 | 17.101 | 1.00 | 20.50 | 6 |
| | ATOM | 3435 | O | ALA | B | 164 | 47.419 | 8.750 | 16.892 | 1.00 | 23.25 | 8 |
| 65 | ATOM | 3436 | CB | ALA | B | 164 | 49.604 | 8.359 | 19.418 | 1.00 | 20.80 | 6 |
| | ATOM | 3437 | N | ASP | B | 165 | 49.612 | 9.237 | 16.440 | 1.00 | 19.12 | 7 |
| | ATOM | 3438 | CA | ASP | B | 165 | 49.190 | 10.233 | 15.409 | 1.00 | 18.46 | 6 |
| | ATOM | 3439 | C | ASP | B | 165 | 48.550 | 9.577 | 14.207 | 1.00 | 22.82 | 6 |
| | ATOM | 3440 | O | ASP | B | 165 | 47.594 | 10.145 | 13.660 | 1.00 | 22.60 | 8 |
| 70 | ATOM | 3441 | CB | ASP | B | 165 | 50.392 | 10.996 | 14.943 | 1.00 | 18.70 | 6 |
| | ATOM | 3442 | CG | ASP | B | 165 | 51.018 | 12.009 | 15.941 | 1.00 | 18.80 | 6 |
| | ATOM | 3443 | OD1 | ASP | B | 165 | 50.354 | 12.300 | 16.916 | 1.00 | 21.84 | 8 |
| | ATOM | 3444 | OD2 | ASP | B | 165 | 52.112 | 12.486 | 15.692 | 1.00 | 21.56 | 8 |
| | ATOM | 3445 | N | MET | B | 166 | 49.185 | 8.526 | 13.694 | 1.00 | 19.28 | 7 |
| | ATOM | 3446 | CA | MET | B | 166 | 48.660 | 7.953 | 12.411 | 1.00 | 20.68 | 6 |

-83-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|----|
| | ATOM | 3447 | C | MET | B | 166 | 47.436 | 7.082 | 12.604 | 1.00 | 21.52 | 6 |
| | ATOM | 3448 | O | MET | B | 166 | 46.935 | 6.605 | 11.577 | 1.00 | 22.25 | 8 |
| | ATOM | 3449 | CB | MET | B | 166 | 49.878 | 7.292 | 11.723 | 1.00 | 17.15 | 6 |
| 5 | ATOM | 3450 | CG | MET | B | 166 | 50.905 | 8.348 | 11.281 | 1.00 | 21.78 | 6 |
| | ATOM | 3451 | SD | MET | B | 166 | 50.266 | 9.743 | 10.357 | 1.00 | 21.48 | 16 |
| | ATOM | 3452 | CE | MET | B | 166 | 49.315 | 9.048 | 8.969 | 1.00 | 22.58 | 6 |
| | ATOM | 3453 | N | GLY | B | 167 | 46.947 | 6.745 | 13.792 | 1.00 | 22.34 | 7 |
| | ATOM | 3454 | CA | GLY | B | 167 | 45.725 | 5.983 | 14.001 | 1.00 | 21.60 | 6 |
| 10 | ATOM | 3455 | C | GLY | B | 167 | 45.804 | 4.480 | 13.881 | 1.00 | 21.23 | 6 |
| | ATOM | 3456 | O | GLY | B | 167 | 44.803 | 3.783 | 13.677 | 1.00 | 19.88 | 8 |
| | ATOM | 3457 | N | PHE | B | 168 | 47.043 | 3.939 | 13.961 | 1.00 | 21.11 | 7 |
| | ATOM | 3458 | CA | PHE | B | 168 | 47.170 | 2.494 | 13.958 | 1.00 | 20.42 | 6 |
| | ATOM | 3459 | C | PHE | B | 168 | 46.553 | 1.828 | 15.193 | 1.00 | 20.83 | 6 |
| 15 | ATOM | 3460 | O | PHE | B | 168 | 46.842 | 2.233 | 16.321 | 1.00 | 22.53 | 8 |
| | ATOM | 3461 | CB | PHE | B | 168 | 48.653 | 2.079 | 13.921 | 1.00 | 21.51 | 6 |
| | ATOM | 3462 | CG | PHE | B | 168 | 49.420 | 2.244 | 12.648 | 1.00 | 21.26 | 6 |
| | ATOM | 3463 | CD1 | PHE | B | 168 | 50.305 | 3.310 | 12.535 | 1.00 | 21.28 | 6 |
| | ATOM | 3464 | CD2 | PHE | B | 168 | 49.352 | 1.351 | 11.604 | 1.00 | 21.16 | 6 |
| 20 | ATOM | 3465 | CE1 | PHE | B | 168 | 51.095 | 3.489 | 11.409 | 1.00 | 22.13 | 6 |
| | ATOM | 3466 | CE2 | PHE | B | 168 | 50.080 | 1.550 | 10.442 | 1.00 | 24.10 | 6 |
| | ATOM | 3467 | CZ | PHE | B | 168 | 50.978 | 2.592 | 10.348 | 1.00 | 20.59 | 6 |
| | ATOM | 3468 | N | ASP | B | 169 | 45.751 | 0.812 | 14.997 | 1.00 | 22.55 | 7 |
| | ATOM | 3469 | CA | ASP | B | 169 | 45.089 | 0.089 | 16.054 | 1.00 | 23.63 | 6 |
| 25 | ATOM | 3470 | C | ASP | B | 169 | 46.010 | -1.072 | 16.556 | 1.00 | 23.14 | 6 |
| | ATOM | 3471 | O | ASP | B | 169 | 45.637 | -2.215 | 16.493 | 1.00 | 23.77 | 8 |
| | ATOM | 3472 | CB | ASP | B | 169 | 43.773 | -0.497 | 15.594 | 1.00 | 27.60 | 6 |
| | ATOM | 3473 | CG | ASP | B | 169 | 42.879 | -1.031 | 16.711 | 1.00 | 30.74 | 6 |
| | ATOM | 3474 | OD1 | ASP | B | 169 | 43.197 | -0.784 | 17.892 | 1.00 | 34.41 | 8 |
| 30 | ATOM | 3475 | OD2 | ASP | B | 169 | 41.884 | -1.685 | 16.342 | 1.00 | 34.81 | 8 |
| | ATOM | 3476 | N | ILE | B | 170 | 47.137 | -0.643 | 17.058 | 1.00 | 20.48 | 7 |
| | ATOM | 3477 | CA | ILE | B | 170 | 48.196 | -1.584 | 17.457 | 1.00 | 19.43 | 6 |
| | ATOM | 3478 | C | ILE | B | 170 | 48.725 | -1.236 | 18.834 | 1.00 | 21.42 | 6 |
| | ATOM | 3479 | O | ILE | B | 170 | 49.048 | -0.083 | 19.071 | 1.00 | 22.91 | 8 |
| 35 | ATOM | 3480 | CB | ILE | B | 170 | 49.351 | -1.526 | 16.434 | 1.00 | 19.13 | 6 |
| | ATOM | 3481 | CG1 | ILE | B | 170 | 48.940 | -1.849 | 14.994 | 1.00 | 21.06 | 6 |
| | ATOM | 3482 | CG2 | ILE | B | 170 | 50.464 | -2.519 | 16.854 | 1.00 | 20.00 | 6 |
| | ATOM | 3483 | CD1 | ILE | B | 170 | 50.054 | -1.568 | 13.974 | 1.00 | 23.10 | 6 |
| | ATOM | 3484 | N | GLU | B | 171 | 48.847 | -2.233 | 19.720 | 1.00 | 20.51 | 7 |
| 40 | ATOM | 3485 | CA | GLU | B | 171 | 49.415 | -1.968 | 21.050 | 1.00 | 22.48 | 6 |
| | ATOM | 3486 | C | GLU | B | 171 | 50.925 | -1.992 | 20.961 | 1.00 | 23.14 | 6 |
| | ATOM | 3487 | O | GLU | B | 171 | 51.470 | -3.024 | 20.518 | 1.00 | 23.79 | 8 |
| | ATOM | 3488 | CB | GLU | B | 171 | 48.824 | -2.974 | 22.034 | 1.00 | 24.29 | 6 |
| | ATOM | 3489 | CG | GLU | B | 171 | 49.506 | -2.861 | 23.391 | 1.00 | 28.59 | 6 |
| 45 | ATOM | 3490 | CD | GLU | B | 171 | 49.089 | -3.843 | 24.453 | 1.00 | 33.66 | 6 |
| | ATOM | 3491 | OE1 | GLU | B | 171 | 48.310 | -4.782 | 24.246 | 1.00 | 34.21 | 8 |
| | ATOM | 3492 | OE2 | GLU | B | 171 | 49.580 | -3.608 | 25.609 | 1.00 | 37.13 | 8 |
| | ATOM | 3493 | N | ILE | B | 172 | 51.637 | -0.956 | 21.410 | 1.00 | 21.22 | 7 |
| | ATOM | 3494 | CA | ILE | B | 172 | 53.093 | -0.965 | 21.349 | 1.00 | 19.30 | 6 |
| 50 | ATOM | 3495 | C | ILE | B | 172 | 53.656 | -1.362 | 22.720 | 1.00 | 24.29 | 6 |
| | ATOM | 3496 | O | ILE | B | 172 | 53.145 | -0.847 | 23.730 | 1.00 | 25.41 | 8 |
| | ATOM | 3497 | CB | ILE | B | 172 | 53.631 | 0.401 | 20.893 | 1.00 | 20.79 | 6 |
| | ATOM | 3498 | CG1 | ILE | B | 172 | 53.086 | 0.809 | 19.509 | 1.00 | 22.57 | 6 |
| | ATOM | 3499 | CG2 | ILE | B | 172 | 55.162 | 0.435 | 20.888 | 1.00 | 22.05 | 6 |
| 55 | ATOM | 3500 | CD1 | ILE | B | 172 | 53.459 | -0.175 | 18.386 | 1.00 | 21.95 | 6 |
| | ATOM | 3501 | N | VAL | B | 173 | 54.392 | -2.471 | 22.752 | 1.00 | 21.27 | 7 |
| | ATOM | 3502 | CA | VAL | B | 173 | 54.895 | -3.034 | 24.024 | 1.00 | 25.99 | 6 |
| | ATOM | 3503 | C | VAL | B | 173 | 56.363 | -2.785 | 24.113 | 1.00 | 25.58 | 6 |
| | ATOM | 3504 | O | VAL | B | 173 | 57.087 | -3.255 | 23.240 | 1.00 | 22.50 | 8 |
| 60 | ATOM | 3505 | CB | VAL | B | 173 | 54.583 | -4.552 | 24.123 | 1.00 | 25.82 | 6 |
| | ATOM | 3506 | CG1 | VAL | B | 173 | 55.242 | -5.122 | 25.406 | 1.00 | 26.85 | 6 |
| | ATOM | 3507 | CG2 | VAL | B | 173 | 53.094 | -4.779 | 24.096 | 1.00 | 27.94 | 6 |
| | ATOM | 3508 | N | GLY | B | 174 | 56.820 | -2.085 | 25.189 | 1.00 | 24.62 | 7 |
| | ATOM | 3509 | CA | GLY | B | 174 | 58.270 | -1.862 | 25.313 | 1.00 | 23.53 | 6 |
| 65 | ATOM | 3510 | C | GLY | B | 174 | 58.740 | -3.002 | 26.282 | 1.00 | 23.91 | 6 |
| | ATOM | 3511 | O | GLY | B | 174 | 57.998 | -3.288 | 27.218 | 1.00 | 26.78 | 8 |
| | ATOM | 3512 | N | VAL | B | 175 | 59.801 | -3.641 | 25.849 | 1.00 | 22.58 | 7 |
| | ATOM | 3513 | CA | VAL | B | 175 | 60.234 | -4.783 | 26.676 | 1.00 | 24.09 | 6 |
| | ATOM | 3514 | C | VAL | B | 175 | 61.523 | -4.341 | 27.430 | 1.00 | 23.90 | 6 |
| 70 | ATOM | 3515 | O | VAL | B | 175 | 62.502 | -4.011 | 26.762 | 1.00 | 24.10 | 8 |
| | ATOM | 3516 | CB | VAL | B | 175 | 60.476 | -6.015 | 25.853 | 1.00 | 24.37 | 6 |
| | ATOM | 3517 | CG1 | VAL | B | 175 | 60.852 | -7.180 | 26.767 | 1.00 | 28.33 | 6 |
| | ATOM | 3518 | CG2 | VAL | B | 175 | 59.219 | -6.353 | 24.984 | 1.00 | 24.52 | 6 |
| | ATOM | 3519 | N | PRO | B | 176 | 61.469 | -4.464 | 28.728 | 1.00 | 28.58 | 7 |
| | ATOM | 3520 | CA | PRO | B | 176 | 62.648 | -4.211 | 29.574 | 1.00 | 32.47 | 6 |

-84-

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|----|
| | ATOM | 3521 | C | PRO | B | 176 | 63.888 | -4.974 | 29.180 | 1.00 | 32.41 | 6 |
| | ATOM | 3522 | O | PRO | B | 176 | 63.831 | -6.135 | 28.746 | 1.00 | 28.92 | 8 |
| | ATOM | 3523 | CB | PRO | B | 176 | 62.159 | -4.588 | 30.980 | 1.00 | 33.03 | 6 |
| 5 | ATOM | 3524 | CG | PRO | B | 176 | 60.685 | -4.380 | 30.922 | 1.00 | 34.15 | 6 |
| | ATOM | 3525 | CD | PRO | B | 176 | 60.320 | -4.916 | 29.543 | 1.00 | 28.09 | 6 |
| | ATOM | 3526 | N | ILE | B | 177 | 65.121 | -4.418 | 29.353 | 1.00 | 31.48 | 7 |
| | ATOM | 3527 | CA | ILE | B | 177 | 66.307 | -5.079 | 28.865 | 1.00 | 32.30 | 6 |
| | ATOM | 3528 | C | ILE | B | 177 | 66.572 | -6.407 | 29.607 | 1.00 | 30.07 | 6 |
| 10 | ATOM | 3529 | O | ILE | B | 177 | 66.054 | -6.698 | 30.686 | 1.00 | 32.04 | 8 |
| | ATOM | 3530 | CB | ILE | B | 177 | 67.641 | -4.292 | 28.903 | 1.00 | 33.70 | 6 |
| | ATOM | 3531 | CG1 | ILE | B | 177 | 68.066 | -3.943 | 30.331 | 1.00 | 33.12 | 6 |
| | ATOM | 3532 | CG2 | ILE | B | 177 | 67.518 | -3.039 | 28.030 | 1.00 | 34.28 | 6 |
| | ATOM | 3533 | CD1 | ILE | B | 177 | 69.430 | -3.243 | 30.349 | 1.00 | 34.81 | 6 |
| 15 | ATOM | 3534 | N | MET | B | 178 | 67.408 | -7.204 | 28.952 | 1.00 | 32.08 | 7 |
| | ATOM | 3535 | CA | MET | B | 178 | 67.674 | -8.503 | 29.572 | 1.00 | 35.37 | 6 |
| | ATOM | 3536 | C | MET | B | 178 | 68.620 | -8.292 | 30.772 | 1.00 | 34.12 | 6 |
| | ATOM | 3537 | O | MET | B | 178 | 69.597 | -7.573 | 30.642 | 1.00 | 31.98 | 8 |
| | ATOM | 3538 | CB | MET | B | 178 | 68.295 | -9.532 | 28.641 | 1.00 | 40.27 | 6 |
| 20 | ATOM | 3539 | CG | MET | B | 178 | 67.437 | -10.819 | 28.679 | 1.00 | 44.21 | 6 |
| | ATOM | 3540 | SD | MET | B | 178 | 68.203 | -12.124 | 27.749 | 1.00 | 51.85 | 16 |
| | ATOM | 3541 | CE | MET | B | 178 | 69.561 | -11.316 | 26.916 | 1.00 | 48.86 | 6 |
| | ATOM | 3542 | N | ARG | B | 179 | 68.313 | -8.994 | 31.814 | 1.00 | 35.69 | 7 |
| | ATOM | 3543 | CA | ARG | B | 179 | 69.085 | -8.847 | 33.060 | 1.00 | 36.43 | 6 |
| 25 | ATOM | 3544 | C | ARG | B | 179 | 69.292 | -10.188 | 33.715 | 1.00 | 37.86 | 6 |
| | ATOM | 3545 | O | ARG | B | 179 | 68.430 | -11.054 | 33.618 | 1.00 | 38.23 | 8 |
| | ATOM | 3546 | CB | ARG | B | 179 | 68.260 | -7.887 | 33.870 | 1.00 | 36.62 | 6 |
| | ATOM | 3547 | CG | ARG | B | 179 | 68.473 | -7.248 | 35.163 | 1.00 | 38.40 | 6 |
| | ATOM | 3548 | CD | ARG | B | 179 | 67.373 | -6.311 | 35.598 | 1.00 | 34.70 | 6 |
| 30 | ATOM | 3549 | NE | ARG | B | 179 | 67.202 | -5.122 | 34.808 | 1.00 | 31.82 | 7 |
| | ATOM | 3550 | CZ | ARG | B | 179 | 68.057 | -4.149 | 34.534 | 1.00 | 32.71 | 6 |
| | ATOM | 3551 | NH1 | ARG | B | 179 | 69.308 | -4.167 | 34.984 | 1.00 | 30.99 | 7 |
| | ATOM | 3552 | NH2 | ARG | B | 179 | 67.715 | -3.067 | 33.831 | 1.00 | 33.25 | 7 |
| | ATOM | 3553 | N | ALA | B | 180 | 70.363 | -10.335 | 34.477 | 1.00 | 36.11 | 7 |
| 35 | ATOM | 3554 | CA | ALA | B | 180 | 70.602 | -11.562 | 35.235 | 1.00 | 36.60 | 6 |
| | ATOM | 3555 | C | ALA | B | 180 | 69.640 | -11.614 | 36.404 | 1.00 | 36.37 | 6 |
| | ATOM | 3556 | O | ALA | B | 180 | 68.929 | -10.685 | 36.743 | 1.00 | 36.44 | 8 |
| | ATOM | 3557 | CB | ALA | B | 180 | 72.048 | -11.541 | 35.689 | 1.00 | 36.08 | 6 |
| | ATOM | 3558 | N | LYS | B | 181 | 69.621 | -12.775 | 37.102 | 1.00 | 37.25 | 7 |
| 40 | ATOM | 3559 | CA | LYS | B | 181 | 68.797 | -12.903 | 38.292 | 1.00 | 38.41 | 6 |
| | ATOM | 3560 | C | LYS | B | 181 | 69.223 | -11.942 | 39.395 | 1.00 | 37.82 | 6 |
| | ATOM | 3561 | O | LYS | B | 181 | 68.366 | -11.482 | 40.158 | 1.00 | 40.11 | 8 |
| | ATOM | 3562 | CB | LYS | B | 181 | 68.862 | -14.317 | 38.895 | 1.00 | 39.54 | 6 |
| | ATOM | 3563 | N | ASP | B | 182 | 70.495 | -11.584 | 39.503 | 1.00 | 36.65 | 7 |
| 45 | ATOM | 3564 | CA | ASP | B | 182 | 70.935 | -10.663 | 40.548 | 1.00 | 35.51 | 6 |
| | ATOM | 3565 | C | ASP | B | 182 | 70.714 | -9.206 | 40.091 | 1.00 | 35.06 | 6 |
| | ATOM | 3566 | O | ASP | B | 182 | 71.004 | -8.303 | 40.868 | 1.00 | 33.11 | 8 |
| | ATOM | 3567 | CB | ASP | B | 182 | 72.392 | -10.861 | 40.981 | 1.00 | 37.04 | 6 |
| | ATOM | 3568 | CG | ASP | B | 182 | 73.414 | -10.661 | 39.890 | 1.00 | 38.43 | 6 |
| 50 | ATOM | 3569 | OD1 | ASP | B | 182 | 73.047 | -10.265 | 38.753 | 1.00 | 38.66 | 8 |
| | ATOM | 3570 | OD2 | ASP | B | 182 | 74.624 | -10.938 | 40.116 | 1.00 | 38.45 | 8 |
| | ATOM | 3571 | N | GLY | B | 183 | 70.283 | -8.992 | 38.840 | 1.00 | 35.23 | 7 |
| | ATOM | 3572 | CA | GLY | B | 183 | 69.907 | -7.618 | 38.467 | 1.00 | 32.81 | 6 |
| | ATOM | 3573 | C | GLY | B | 183 | 70.883 | -7.003 | 37.494 | 1.00 | 33.61 | 6 |
| 55 | ATOM | 3574 | O | GLY | B | 183 | 70.523 | -5.956 | 36.928 | 1.00 | 33.06 | 8 |
| | ATOM | 3575 | N | LEU | B | 184 | 72.029 | -7.592 | 37.220 | 1.00 | 31.99 | 7 |
| | ATOM | 3576 | CA | LEU | B | 184 | 72.977 | -7.004 | 36.286 | 1.00 | 32.29 | 6 |
| | ATOM | 3577 | C | LEU | B | 184 | 72.517 | -7.011 | 34.826 | 1.00 | 33.46 | 6 |
| | ATOM | 3578 | O | LEU | B | 184 | 72.300 | -8.130 | 34.314 | 1.00 | 32.16 | 8 |
| 60 | ATOM | 3579 | CB | LEU | B | 184 | 74.325 | -7.737 | 36.370 | 1.00 | 32.38 | 6 |
| | ATOM | 3580 | CG | LEU | B | 184 | 75.481 | -7.019 | 35.655 | 1.00 | 32.34 | 6 |
| | ATOM | 3581 | CD1 | LEU | B | 184 | 75.643 | -5.559 | 36.125 | 1.00 | 34.61 | 6 |
| | ATOM | 3582 | CD2 | LEU | B | 184 | 76.748 | -7.838 | 35.853 | 1.00 | 34.57 | 6 |
| | ATOM | 3583 | N | ALA | B | 185 | 72.466 | -5.818 | 34.204 | 1.00 | 32.96 | 7 |
| 65 | ATOM | 3584 | CA | ALA | B | 185 | 72.099 | -5.821 | 32.780 | 1.00 | 33.17 | 6 |
| | ATOM | 3585 | C | ALA | B | 185 | 73.053 | -6.670 | 31.950 | 1.00 | 35.69 | 6 |
| | ATOM | 3586 | O | ALA | B | 185 | 74.281 | -6.510 | 32.057 | 1.00 | 35.57 | 8 |
| | ATOM | 3587 | CB | ALA | B | 185 | 72.076 | -4.368 | 32.316 | 1.00 | 29.95 | 6 |
| | ATOM | 1443 | N | LEU | B | 186 | 72.752 | -7.823 | 31.203 | 1.00 | 16.87 | |
| 70 | ATOM | 1444 | CA | LEU | B | 186 | 73.699 | -8.676 | 30.476 | 1.00 | 16.99 | |
| | ATOM | 1445 | C | LEU | B | 186 | 74.354 | -7.793 | 29.406 | 1.00 | 17.67 | |
| | ATOM | 1446 | O | LEU | B | 186 | 73.662 | -7.050 | 28.666 | 1.00 | 20.34 | |
| | ATOM | 1447 | CB | LEU | B | 186 | 73.001 | -9.890 | 29.872 | 1.00 | 16.87 | |
| | ATOM | 1448 | CG | LEU | B | 186 | 72.315 | -10.841 | 30.851 | 1.00 | 18.67 | |
| | ATOM | 1449 | CD1 | LEU | B | 186 | 71.803 | -12.062 | 30.097 | 1.00 | 20.67 | |

-85-

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| | ATOM | 1450 | CD2 | LEU | B | 186 | 73.289 | -11.257 | 31.936 | 1.00 | 17.31 | |
| | ATOM | 1451 | N | SER | B | 187 | 75.650 | -7.991 | 29.285 | 1.00 | 18.83 | |
| | ATOM | 1452 | CA | SER | B | 187 | 76.407 | -7.179 | 28.327 | 1.00 | 17.18 | |
| 5 | ATOM | 1453 | C | SER | B | 187 | 77.754 | -7.771 | 28.079 | 1.00 | 17.64 | |
| | ATOM | 1454 | O | SER | B | 187 | 78.405 | -8.305 | 28.987 | 1.00 | 18.63 | |
| | ATOM | 1455 | CB | SER | B | 187 | 76.597 | -5.762 | 28.933 | 1.00 | 20.23 | |
| | ATOM | 1456 | OG | SER | B | 187 | 77.485 | -4.989 | 28.093 | 1.00 | 20.91 | |
| | ATOM | 1457 | N | SER | B | 188 | 78.290 | -7.564 | 26.832 | 1.00 | 17.55 | |
| 10 | ATOM | 1458 | CA | SER | B | 188 | 79.706 | -7.917 | 26.649 | 1.00 | 17.70 | |
| | ATOM | 1459 | C | SER | B | 188 | 80.653 | -7.182 | 27.579 | 1.00 | 17.74 | |
| | ATOM | 1460 | O | SER | B | 188 | 81.764 | -7.648 | 27.944 | 1.00 | 18.92 | |
| | ATOM | 1461 | CB | SER | B | 188 | 80.127 | -7.598 | 25.196 | 1.00 | 19.73 | |
| | ATOM | 1462 | OG | SER | B | 188 | 79.893 | -6.208 | 24.915 | 1.00 | 20.84 | |
| 15 | ATOM | 1463 | N | ARG | B | 189 | 80.298 | -6.012 | 28.096 | 1.00 | 18.16 | |
| | ATOM | 1464 | CA | ARG | B | 189 | 81.104 | -5.205 | 28.988 | 1.00 | 19.85 | |
| | ATOM | 1465 | C | ARG | B | 189 | 81.386 | -5.909 | 30.311 | 1.00 | 20.33 | |
| | ATOM | 1466 | O | ARG | B | 189 | 82.356 | -5.612 | 30.969 | 1.00 | 21.91 | |
| | ATOM | 1467 | CB | ARG | B | 189 | 80.426 | -3.848 | 29.284 | 1.00 | 20.55 | |
| 20 | ATOM | 1468 | CG | ARG | B | 189 | 80.245 | -3.075 | 27.973 | 1.00 | 22.89 | |
| | ATOM | 1469 | CD | ARG | B | 189 | 79.609 | -1.707 | 28.273 | 1.00 | 23.21 | |
| | ATOM | 1470 | NE | ARG | B | 189 | 79.461 | -1.073 | 26.939 | 1.00 | 25.97 | |
| | ATOM | 1471 | CZ | ARG | B | 189 | 79.880 | 0.157 | 26.683 | 1.00 | 28.29 | |
| | ATOM | 1472 | NH1 | ARG | B | 189 | 80.387 | 0.915 | 27.617 | 1.00 | 26.60 | |
| 25 | ATOM | 1473 | NH2 | ARG | B | 189 | 79.714 | 0.627 | 25.429 | 1.00 | 28.41 | |
| | ATOM | 1474 | N | ASN | B | 190 | 80.441 | -6.790 | 30.763 | 1.00 | 19.42 | |
| | ATOM | 1475 | CA | ASN | B | 190 | 80.639 | -7.442 | 32.041 | 1.00 | 19.64 | |
| | ATOM | 1476 | C | ASN | B | 190 | 81.891 | -8.271 | 32.059 | 1.00 | 22.61 | |
| | ATOM | 1477 | O | ASN | B | 190 | 82.467 | -8.717 | 33.097 | 1.00 | 23.27 | |
| 30 | ATOM | 1478 | CB | ASN | B | 190 | 79.437 | -8.347 | 32.355 | 1.00 | 19.54 | |
| | ATOM | 1479 | CG | ASN | B | 190 | 78.168 | -7.518 | 32.494 | 1.00 | 21.41 | |
| | ATOM | 1480 | OD1 | ASN | B | 190 | 77.045 | -8.077 | 32.323 | 1.00 | 21.40 | |
| | ATOM | 1481 | ND2 | ASN | B | 190 | 78.310 | -6.244 | 32.814 | 1.00 | 19.16 | |
| | ATOM | 1497 | N | GLY | B | 191 | 82.333 | -8.712 | 30.735 | 1.00 | 27.44 | |
| 35 | ATOM | 1498 | CA | GLY | B | 191 | 83.554 | -9.514 | 30.632 | 1.00 | 28.04 | |
| | ATOM | 1499 | C | GLY | B | 191 | 84.823 | -8.796 | 31.035 | 1.00 | 29.70 | |
| | ATOM | 1500 | O | GLY | B | 191 | 85.815 | -9.487 | 31.266 | 1.00 | 31.47 | |
| | ATOM | 1482 | N | TYR | B | 192 | 84.825 | -7.501 | 31.228 | 1.00 | 26.92 | |
| | ATOM | 1483 | CA | TYR | B | 192 | 86.032 | -6.786 | 31.629 | 1.00 | 29.88 | |
| 40 | ATOM | 1484 | C | TYR | B | 192 | 86.054 | -6.581 | 33.125 | 1.00 | 29.91 | |
| | ATOM | 1485 | O | TYR | B | 192 | 87.053 | -5.998 | 33.601 | 1.00 | 34.28 | |
| | ATOM | 1486 | CB | TYR | B | 192 | 86.154 | -5.424 | 30.922 | 1.00 | 30.32 | |
| | ATOM | 1487 | CG | TYR | B | 192 | 86.340 | -5.687 | 29.438 | 1.00 | 32.17 | |
| | ATOM | 1488 | CD1 | TYR | B | 192 | 85.211 | -5.943 | 28.667 | 1.00 | 32.38 | |
| 45 | ATOM | 1489 | CD2 | TYR | B | 192 | 87.596 | -5.764 | 28.842 | 1.00 | 34.00 | |
| | ATOM | 1490 | CE1 | TYR | B | 192 | 85.313 | -6.234 | 27.337 | 1.00 | 35.21 | |
| | ATOM | 1491 | CE2 | TYR | B | 192 | 87.703 | -6.056 | 27.486 | 1.00 | 34.55 | |
| | ATOM | 1492 | CZ | TYR | B | 192 | 86.578 | -6.276 | 26.747 | 1.00 | 36.66 | |
| | ATOM | 1493 | OH | TYR | B | 192 | 86.631 | -6.577 | 25.395 | 1.00 | 38.33 | |
| 50 | ATOM | 1494 | N | LEU | B | 193 | 85.033 | -7.028 | 33.865 | 1.00 | 28.20 | |
| | ATOM | 1495 | CA | LEU | B | 193 | 85.075 | -6.900 | 35.299 | 1.00 | 26.63 | |
| | ATOM | 1496 | C | LEU | B | 193 | 85.870 | -7.994 | 35.986 | 1.00 | 27.15 | |
| | ATOM | 1497 | O | LEU | B | 193 | 85.690 | -9.155 | 35.614 | 1.00 | 28.28 | |
| | ATOM | 1498 | CB | LEU | B | 193 | 83.651 | -6.979 | 35.888 | 1.00 | 26.20 | |
| 55 | ATOM | 1499 | CG | LEU | B | 193 | 82.648 | -5.971 | 35.339 | 1.00 | 25.58 | |
| | ATOM | 1500 | CD1 | LEU | B | 193 | 81.223 | -6.375 | 35.649 | 1.00 | 24.08 | |
| | ATOM | 1501 | CD2 | LEU | B | 193 | 82.909 | -4.563 | 35.910 | 1.00 | 27.77 | |
| | ATOM | 1502 | N | THR | B | 194 | 86.596 | -7.704 | 37.090 | 1.00 | 28.42 | |
| | ATOM | 1503 | CA | THR | B | 194 | 87.177 | -8.819 | 37.838 | 1.00 | 27.62 | |
| 60 | ATOM | 1504 | C | THR | B | 194 | 86.087 | -9.564 | 38.585 | 1.00 | 25.74 | |
| | ATOM | 1505 | O | THR | B | 194 | 84.983 | -8.990 | 38.712 | 1.00 | 26.48 | |
| | ATOM | 1506 | CB | THR | B | 194 | 88.236 | -8.313 | 38.835 | 1.00 | 29.34 | |
| | ATOM | 1507 | OG1 | THR | B | 194 | 87.611 | -7.354 | 39.693 | 1.00 | 30.55 | |
| | ATOM | 1508 | CG2 | THR | B | 194 | 89.370 | -7.647 | 38.064 | 1.00 | 32.65 | |
| 65 | ATOM | 3620 | N | ALA | B | 195 | 86.095 | -11.397 | 38.739 | 1.00 | 45.01 | 7 |
| | ATOM | 3621 | CA | ALA | B | 195 | 85.137 | -12.052 | 39.619 | 1.00 | 45.61 | 6 |
| | ATOM | 3622 | C | ALA | B | 195 | 84.702 | -11.095 | 40.732 | 1.00 | 46.90 | 6 |
| | ATOM | 3623 | O | ALA | B | 195 | 83.510 | -11.093 | 41.082 | 1.00 | 45.91 | 8 |
| | ATOM | 3624 | CB | ALA | B | 195 | 85.717 | -13.336 | 40.196 | 1.00 | 46.79 | 6 |
| | ATOM | 3625 | N | GLU | B | 196 | 85.603 | -10.280 | 41.278 | 1.00 | 47.33 | 7 |
| 70 | ATOM | 3626 | CA | GLU | B | 196 | 85.242 | -9.350 | 42.330 | 1.00 | 48.34 | 6 |
| | ATOM | 3627 | C | GLU | B | 196 | 84.313 | -8.252 | 41.828 | 1.00 | 46.99 | 6 |
| | ATOM | 3628 | O | GLU | B | 196 | 83.325 | -7.912 | 42.497 | 1.00 | 47.72 | 8 |
| | ATOM | 3629 | CB | GLU | B | 196 | 86.459 | -8.634 | 42.959 | 1.00 | 52.20 | 6 |
| | ATOM | 3630 | CG | GLU | B | 196 | 86.011 | -7.646 | 44.018 | 1.00 | 56.19 | 6 |

-86-

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|----|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| | ATOM | 3631 | CD | GLU | B | 196 | 86.989 | -6.639 | 44.543 | 1.00 | 59.41 | 6 |
| | ATOM | 3632 | OE1 | GLU | B | 196 | 88.104 | -6.474 | 43.993 | 1.00 | 61.45 | 8 |
| | ATOM | 3633 | OE2 | GLU | B | 196 | 86.639 | -5.966 | 45.555 | 1.00 | 61.84 | 8 |
| 5 | ATOM | 3634 | N | GLN | B | 197 | 84.641 | -7.664 | 40.687 | 1.00 | 44.75 | 7 |
| | ATOM | 3635 | CA | GLN | B | 197 | 83.801 | -6.624 | 40.095 | 1.00 | 43.46 | 6 |
| | ATOM | 3636 | C | GLN | B | 197 | 82.428 | -7.188 | 39.782 | 1.00 | 42.72 | 6 |
| | ATOM | 3637 | O | GLN | B | 197 | 81.425 | -6.478 | 39.983 | 1.00 | 41.97 | 8 |
| | ATOM | 3638 | CB | GLN | B | 197 | 84.430 | -6.018 | 38.832 | 1.00 | 43.86 | 6 |
| 10 | ATOM | 3639 | CG | GLN | B | 197 | 85.754 | -5.346 | 39.203 | 1.00 | 46.24 | 6 |
| | ATOM | 3640 | CD | GLN | B | 197 | 86.485 | -4.709 | 38.047 | 1.00 | 48.63 | 6 |
| | ATOM | 3641 | OE1 | GLN | B | 197 | 86.387 | -5.148 | 36.902 | 1.00 | 50.12 | 8 |
| | ATOM | 3642 | NE2 | GLN | B | 197 | 87.247 | -3.655 | 38.397 | 1.00 | 49.65 | 7 |
| | ATOM | 3643 | N | ARG | B | 198 | 82.339 | -8.436 | 39.342 | 1.00 | 40.11 | 7 |
| 15 | ATOM | 3644 | CA | ARG | B | 198 | 81.024 | -9.023 | 39.025 | 1.00 | 40.65 | 6 |
| | ATOM | 3645 | C | ARG | B | 198 | 80.231 | -9.134 | 40.321 | 1.00 | 40.50 | 6 |
| | ATOM | 3646 | O | ARG | B | 198 | 79.001 | -9.070 | 40.226 | 1.00 | 40.26 | 8 |
| | ATOM | 3647 | CB | ARG | B | 198 | 81.196 | -10.331 | 38.255 | 1.00 | 38.75 | 6 |
| | ATOM | 3648 | CG | ARG | B | 198 | 79.950 | -11.169 | 37.980 | 1.00 | 40.23 | 6 |
| 20 | ATOM | 3649 | CD | ARG | B | 198 | 78.984 | -10.360 | 37.114 | 1.00 | 38.56 | 6 |
| | ATOM | 3650 | NE | ARG | B | 198 | 77.712 | -10.999 | 36.860 | 1.00 | 40.33 | 7 |
| | ATOM | 3651 | CZ | ARG | B | 198 | 76.685 | -10.913 | 37.703 | 1.00 | 38.73 | 6 |
| | ATOM | 3652 | NH1 | ARG | B | 198 | 76.828 | -10.212 | 38.843 | 1.00 | 37.38 | 7 |
| | ATOM | 3653 | NH2 | ARG | B | 198 | 75.530 | -11.506 | 37.383 | 1.00 | 39.11 | 7 |
| 25 | ATOM | 3654 | N | LYS | B | 199 | 80.821 | -9.198 | 41.506 | 1.00 | 40.18 | 7 |
| | ATOM | 3655 | CA | LYS | B | 199 | 80.067 | -9.237 | 42.738 | 1.00 | 41.84 | 6 |
| | ATOM | 3656 | C | LYS | B | 199 | 79.519 | -7.843 | 43.083 | 1.00 | 39.14 | 6 |
| | ATOM | 3657 | O | LYS | B | 199 | 78.440 | -7.806 | 43.660 | 1.00 | 39.85 | 8 |
| | ATOM | 3658 | CB | LYS | B | 199 | 80.852 | -9.706 | 43.969 | 1.00 | 44.70 | 6 |
| 30 | ATOM | 3659 | CG | LYS | B | 199 | 81.675 | -10.963 | 43.783 | 1.00 | 48.43 | 6 |
| | ATOM | 3660 | CD | LYS | B | 199 | 82.186 | -11.540 | 45.087 | 1.00 | 50.67 | 6 |
| | ATOM | 3661 | CE | LYS | B | 199 | 82.837 | -10.559 | 46.037 | 1.00 | 52.79 | 6 |
| | ATOM | 3662 | NZ | LYS | B | 199 | 84.285 | -10.286 | 45.751 | 1.00 | 55.36 | 7 |
| | ATOM | 3663 | N | ILE | B | 200 | 80.245 | -6.791 | 42.754 | 1.00 | 36.48 | 7 |
| 35 | ATOM | 3664 | CA | ILE | B | 200 | 79.815 | -5.425 | 43.013 | 1.00 | 36.30 | 6 |
| | ATOM | 3665 | C | ILE | B | 200 | 78.867 | -4.836 | 41.964 | 1.00 | 34.09 | 6 |
| | ATOM | 3666 | O | ILE | B | 200 | 77.970 | -4.048 | 42.300 | 1.00 | 31.98 | 8 |
| | ATOM | 3667 | CB | ILE | B | 200 | 81.036 | -4.477 | 43.052 | 1.00 | 37.30 | 6 |
| | ATOM | 3668 | CG1 | ILE | B | 200 | 81.938 | -4.835 | 44.261 | 1.00 | 39.39 | 6 |
| 40 | ATOM | 3669 | CG2 | ILE | B | 200 | 80.668 | -2.995 | 43.087 | 1.00 | 38.32 | 6 |
| | ATOM | 3670 | CD1 | ILE | B | 200 | 83.228 | -4.024 | 44.171 | 1.00 | 39.23 | 6 |
| | ATOM | 3671 | N | ALA | B | 201 | 78.923 | -5.343 | 40.749 | 1.00 | 31.89 | 7 |
| | ATOM | 3672 | CA | ALA | B | 201 | 78.199 | -4.790 | 39.605 | 1.00 | 30.33 | 6 |
| | ATOM | 3673 | C | ALA | B | 201 | 76.683 | -4.738 | 39.757 | 1.00 | 30.26 | 6 |
| 45 | ATOM | 3674 | O | ALA | B | 201 | 76.126 | -3.736 | 39.270 | 1.00 | 28.19 | 8 |
| | ATOM | 3675 | CB | ALA | B | 201 | 78.588 | -5.549 | 38.327 | 1.00 | 31.33 | 6 |
| | ATOM | 3676 | N | PRO | B | 202 | 75.978 | -5.632 | 40.395 | 1.00 | 29.89 | 7 |
| | ATOM | 3677 | CA | PRO | B | 202 | 74.538 | -5.483 | 40.618 | 1.00 | 31.17 | 6 |
| | ATOM | 3678 | C | PRO | B | 202 | 74.130 | -4.220 | 41.350 | 1.00 | 30.89 | 6 |
| 50 | ATOM | 3679 | O | PRO | B | 202 | 72.942 | -3.842 | 41.356 | 1.00 | 33.70 | 8 |
| | ATOM | 3680 | CB | PRO | B | 202 | 74.171 | -6.714 | 41.422 | 1.00 | 31.80 | 6 |
| | ATOM | 3681 | CG | PRO | B | 202 | 75.203 | -7.727 | 41.041 | 1.00 | 32.51 | 6 |
| | ATOM | 3682 | CD | PRO | B | 202 | 76.485 | -6.926 | 40.935 | 1.00 | 30.92 | 6 |
| | ATOM | 3683 | N | GLY | B | 203 | 75.003 | -3.520 | 42.079 | 1.00 | 30.61 | 7 |
| 55 | ATOM | 3684 | CA | GLY | B | 203 | 74.724 | -2.274 | 42.775 | 1.00 | 29.71 | 6 |
| | ATOM | 3685 | C | GLY | B | 203 | 74.185 | -1.180 | 41.844 | 1.00 | 29.14 | 6 |
| | ATOM | 3686 | O | GLY | B | 203 | 73.382 | -0.333 | 42.278 | 1.00 | 27.39 | 8 |
| | ATOM | 3687 | N | LEU | B | 204 | 74.569 | -1.208 | 40.562 | 1.00 | 26.29 | 7 |
| | ATOM | 3688 | CA | LEU | B | 204 | 74.116 | -0.193 | 39.634 | 1.00 | 27.87 | 6 |
| 60 | ATOM | 3689 | C | LEU | B | 204 | 72.595 | -0.279 | 39.482 | 1.00 | 26.50 | 6 |
| | ATOM | 3690 | O | LEU | B | 204 | 71.878 | 0.736 | 39.532 | 1.00 | 26.32 | 8 |
| | ATOM | 3691 | CB | LEU | B | 204 | 74.789 | -0.294 | 38.259 | 1.00 | 28.45 | 6 |
| | ATOM | 3692 | CG | LEU | B | 204 | 74.362 | 0.731 | 37.212 | 1.00 | 29.87 | 6 |
| | ATOM | 3693 | CD1 | LEU | B | 204 | 74.600 | 2.168 | 37.697 | 1.00 | 31.40 | 6 |
| 65 | ATOM | 3694 | CD2 | LEU | B | 204 | 75.087 | 0.559 | 35.887 | 1.00 | 32.44 | 6 |
| | ATOM | 3695 | N | TYR | B | 205 | 72.132 | -1.509 | 39.245 | 1.00 | 26.81 | 7 |
| | ATOM | 3696 | CA | TYR | B | 205 | 70.667 | -1.619 | 39.081 | 1.00 | 28.26 | 6 |
| | ATOM | 3697 | C | TYR | B | 205 | 69.946 | -1.322 | 40.382 | 1.00 | 28.28 | 6 |
| | ATOM | 3698 | O | TYR | B | 205 | 68.816 | -0.829 | 40.340 | 1.00 | 27.87 | 8 |
| 70 | ATOM | 3699 | CB | TYR | B | 205 | 70.328 | -2.995 | 38.524 | 1.00 | 27.88 | 6 |
| | ATOM | 3700 | CG | TYR | B | 205 | 68.848 | -3.144 | 38.265 | 1.00 | 30.23 | 6 |
| | ATOM | 3701 | CD1 | TYR | B | 205 | 68.193 | -2.323 | 37.360 | 1.00 | 30.41 | 6 |
| | ATOM | 3702 | CD2 | TYR | B | 205 | 68.111 | -4.106 | 38.935 | 1.00 | 32.30 | 6 |
| | ATOM | 3703 | CE1 | TYR | B | 205 | 66.838 | -2.493 | 37.115 | 1.00 | 31.17 | 6 |
| | ATOM | 3704 | CE2 | TYR | B | 205 | 66.743 | -4.304 | 38.698 | 1.00 | 32.16 | 6 |

-87-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3705 | CZ | TYR | B | 205 | 66.134 | -3.480 | 37.784 | 1.00 | 33.79 | 6 |
| | ATOM | 3706 | OH | TYR | B | 205 | 64.774 | -3.587 | 37.529 | 1.00 | 36.69 | 8 |
| | ATOM | 3707 | N | LYS | B | 206 | 70.554 | -1.567 | 41.568 | 1.00 | 27.79 | 7 |
| 5 | ATOM | 3708 | CA | LYS | B | 206 | 69.949 | -1.137 | 42.812 | 1.00 | 28.48 | 6 |
| | ATOM | 3709 | C | LYS | B | 206 | 69.794 | 0.379 | 42.849 | 1.00 | 26.89 | 6 |
| | ATOM | 3710 | O | LYS | B | 206 | 68.729 | 0.847 | 43.295 | 1.00 | 26.06 | 8 |
| | ATOM | 3711 | CB | LYS | B | 206 | 70.814 | -1.650 | 44.005 | 1.00 | 31.12 | 6 |
| | ATOM | 3712 | CG | LYS | B | 206 | 70.702 | -3.191 | 44.056 | 1.00 | 35.12 | 6 |
| 10 | ATOM | 3713 | CD | LYS | B | 206 | 71.439 | -3.803 | 45.235 | 1.00 | 38.80 | 6 |
| | ATOM | 3714 | CE | LYS | B | 206 | 71.267 | -5.329 | 45.230 | 1.00 | 41.11 | 6 |
| | ATOM | 3715 | NZ | LYS | B | 206 | 72.055 | -5.939 | 46.361 | 1.00 | 44.45 | 7 |
| | ATOM | 3716 | N | VAL | B | 207 | 70.786 | 1.151 | 42.450 | 1.00 | 24.10 | 7 |
| | ATOM | 3717 | CA | VAL | B | 207 | 70.698 | 2.623 | 42.437 | 1.00 | 23.57 | 6 |
| 15 | ATOM | 3718 | C | VAL | B | 207 | 69.692 | 3.075 | 41.353 | 1.00 | 25.00 | 6 |
| | ATOM | 3719 | O | VAL | B | 207 | 68.785 | 3.854 | 41.709 | 1.00 | 25.30 | 8 |
| | ATOM | 3720 | CB | VAL | B | 207 | 72.075 | 3.263 | 42.273 | 1.00 | 25.80 | 6 |
| | ATOM | 3721 | CG1 | VAL | B | 207 | 71.998 | 4.765 | 42.088 | 1.00 | 24.61 | 6 |
| | ATOM | 3722 | CG2 | VAL | B | 207 | 72.941 | 2.900 | 43.507 | 1.00 | 26.07 | 6 |
| 20 | ATOM | 3723 | N | LEU | B | 208 | 69.679 | 2.455 | 40.200 | 1.00 | 25.37 | 7 |
| | ATOM | 3724 | CA | LEU | B | 208 | 68.640 | 2.782 | 39.185 | 1.00 | 25.10 | 6 |
| | ATOM | 3725 | C | LEU | B | 208 | 67.243 | 2.553 | 39.694 | 1.00 | 24.92 | 6 |
| | ATOM | 3726 | O | LEU | B | 208 | 66.280 | 3.338 | 39.468 | 1.00 | 25.42 | 8 |
| | ATOM | 3727 | CB | LEU | B | 208 | 68.989 | 1.910 | 37.985 | 1.00 | 26.66 | 6 |
| | ATOM | 3728 | CG | LEU | B | 208 | 68.261 | 2.079 | 36.661 | 1.00 | 30.34 | 6 |
| 25 | ATOM | 3729 | CD1 | LEU | B | 208 | 68.389 | 3.525 | 36.163 | 1.00 | 32.04 | 6 |
| | ATOM | 3730 | CD2 | LEU | B | 208 | 68.793 | 1.084 | 35.646 | 1.00 | 31.70 | 6 |
| | ATOM | 3731 | N | SER | B | 209 | 67.019 | 1.416 | 40.355 | 1.00 | 26.22 | 7 |
| | ATOM | 3732 | CA | SER | B | 209 | 65.726 | 1.035 | 40.907 | 1.00 | 29.64 | 6 |
| 30 | ATOM | 3733 | C | SER | B | 209 | 65.293 | 2.025 | 41.988 | 1.00 | 30.28 | 6 |
| | ATOM | 3734 | O | SER | B | 209 | 64.107 | 2.380 | 42.055 | 1.00 | 30.20 | 8 |
| | ATOM | 3735 | CB | SER | B | 209 | 65.710 | -0.386 | 41.480 | 1.00 | 30.00 | 6 |
| | ATOM | 3736 | OG | SER | B | 209 | 65.923 | -1.312 | 40.425 | 1.00 | 32.79 | 8 |
| | ATOM | 3737 | N | SER | B | 210 | 66.262 | 2.526 | 42.772 | 1.00 | 29.87 | 7 |
| 35 | ATOM | 3738 | CA | SER | B | 210 | 65.938 | 3.533 | 43.764 | 1.00 | 30.73 | 6 |
| | ATOM | 3739 | C | SER | B | 210 | 65.469 | 4.839 | 43.141 | 1.00 | 28.63 | 6 |
| | ATOM | 3740 | O | SER | B | 210 | 64.551 | 5.481 | 43.694 | 1.00 | 30.02 | 8 |
| | ATOM | 3741 | CB | SER | B | 210 | 67.171 | 3.837 | 44.652 | 1.00 | 33.65 | 6 |
| | ATOM | 3742 | OG | SER | B | 210 | 66.847 | 4.965 | 45.451 | 1.00 | 38.88 | 8 |
| 40 | ATOM | 3743 | N | ILE | B | 211 | 66.115 | 5.259 | 42.067 | 1.00 | 26.67 | 7 |
| | ATOM | 3744 | CA | ILE | B | 211 | 65.727 | 6.462 | 41.337 | 1.00 | 26.97 | 6 |
| | ATOM | 3745 | C | ILE | B | 211 | 64.283 | 6.278 | 40.860 | 1.00 | 29.84 | 6 |
| | ATOM | 3746 | O | ILE | B | 211 | 63.426 | 7.151 | 41.011 | 1.00 | 29.98 | 8 |
| | ATOM | 3747 | CB | ILE | B | 211 | 66.584 | 6.759 | 40.124 | 1.00 | 26.70 | 6 |
| 45 | ATOM | 3748 | CG1 | ILE | B | 211 | 68.031 | 7.036 | 40.607 | 1.00 | 26.03 | 6 |
| | ATOM | 3749 | CG2 | ILE | B | 211 | 66.046 | 7.935 | 39.290 | 1.00 | 27.20 | 6 |
| | ATOM | 3750 | CD1 | ILE | B | 211 | 69.081 | 7.179 | 39.551 | 1.00 | 25.43 | 6 |
| | ATOM | 3751 | N | ALA | B | 212 | 64.062 | 5.111 | 40.250 | 1.00 | 29.63 | 7 |
| | ATOM | 3752 | CA | ALA | B | 212 | 62.703 | 4.840 | 39.732 | 1.00 | 31.76 | 6 |
| 50 | ATOM | 3753 | C | ALA | B | 212 | 61.680 | 4.874 | 40.827 | 1.00 | 33.70 | 6 |
| | ATOM | 3754 | O | ALA | B | 212 | 60.601 | 5.488 | 40.669 | 1.00 | 35.70 | 8 |
| | ATOM | 3755 | CB | ALA | B | 212 | 62.713 | 3.477 | 39.041 | 1.00 | 30.18 | 6 |
| | ATOM | 3756 | N | ASP | B | 213 | 61.985 | 4.267 | 41.976 | 1.00 | 35.57 | 7 |
| | ATOM | 3757 | CA | ASP | B | 213 | 61.051 | 4.267 | 43.097 | 1.00 | 37.44 | 6 |
| | ATOM | 3758 | C | ASP | B | 213 | 60.766 | 5.705 | 43.541 | 1.00 | 38.51 | 6 |
| 55 | ATOM | 3759 | O | ASP | B | 213 | 59.588 | 5.981 | 43.821 | 1.00 | 39.54 | 8 |
| | ATOM | 3760 | CB | ASP | B | 213 | 61.540 | 3.469 | 44.294 | 1.00 | 40.83 | 6 |
| | ATOM | 3761 | CG | ASP | B | 213 | 61.594 | 1.978 | 44.075 | 1.00 | 43.42 | 6 |
| | ATOM | 3762 | OD1 | ASP | B | 213 | 60.952 | 1.468 | 43.127 | 1.00 | 44.23 | 8 |
| 60 | ATOM | 3763 | OD2 | ASP | B | 213 | 62.266 | 1.294 | 44.889 | 1.00 | 45.13 | 8 |
| | ATOM | 3764 | N | LYS | B | 214 | 61.739 | 6.605 | 43.622 | 1.00 | 36.89 | 7 |
| | ATOM | 3765 | CA | LYS | B | 214 | 61.439 | 7.980 | 44.023 | 1.00 | 37.14 | 6 |
| | ATOM | 3766 | C | LYS | B | 214 | 60.553 | 8.695 | 43.015 | 1.00 | 38.10 | 6 |
| | ATOM | 3767 | O | LYS | B | 214 | 59.689 | 9.521 | 43.354 | 1.00 | 38.08 | 8 |
| 65 | ATOM | 3768 | CB | LYS | B | 214 | 62.734 | 8.783 | 44.210 | 1.00 | 35.35 | 6 |
| | ATOM | 3769 | CG | LYS | B | 214 | 63.592 | 8.274 | 45.353 | 1.00 | 34.18 | 6 |
| | ATOM | 3770 | CD | LYS | B | 214 | 64.924 | 9.016 | 45.447 | 1.00 | 33.76 | 6 |
| | ATOM | 3771 | CE | LYS | B | 214 | 65.708 | 8.660 | 46.703 | 1.00 | 35.46 | 6 |
| | ATOM | 3772 | NZ | LYS | B | 214 | 66.968 | 9.471 | 46.836 | 1.00 | 33.81 | 7 |
| 70 | ATOM | 3773 | N | LEU | B | 215 | 60.824 | 8.468 | 41.720 | 1.00 | 37.41 | 7 |
| | ATOM | 3774 | CA | LEU | B | 215 | 60.005 | 9.116 | 40.679 | 1.00 | 38.52 | 6 |
| | ATOM | 3775 | C | LEU | B | 215 | 58.575 | 8.587 | 40.776 | 1.00 | 41.72 | 6 |
| | ATOM | 3776 | O | LEU | B | 215 | 57.606 | 9.372 | 40.631 | 1.00 | 41.98 | 8 |
| | ATOM | 3777 | CB | LEU | B | 215 | 60.604 | 8.904 | 39.310 | 1.00 | 37.43 | 6 |
| | ATOM | 3778 | CG | LEU | B | 215 | 61.897 | 9.594 | 38.900 | 1.00 | 36.45 | 6 |

-88-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3779 | CD1 | LEU | B | 215 | 62.313 | 9.105 | 37.529 | 1.00 | 36.60 | 6 |
| | ATOM | 3780 | CD2 | LEU | B | 215 | 61.767 | 11.119 | 38.869 | 1.00 | 37.66 | 6 |
| | ATOM | 3781 | N | GLN | B | 216 | 58.409 | 7.300 | 41.061 | 1.00 | 42.52 | 7 |
| 5 | ATOM | 3782 | CA | GLN | B | 216 | 57.077 | 6.739 | 41.231 | 1.00 | 46.61 | 6 |
| | ATOM | 3783 | C | GLN | B | 216 | 56.353 | 7.337 | 42.439 | 1.00 | 47.19 | 6 |
| | ATOM | 3784 | O | GLN | B | 216 | 55.125 | 7.438 | 42.427 | 1.00 | 48.78 | 8 |
| | ATOM | 3785 | CB | GLN | B | 216 | 57.069 | 5.232 | 41.449 | 1.00 | 48.29 | 6 |
| | ATOM | 3786 | CG | GLN | B | 216 | 57.290 | 4.444 | 40.180 | 1.00 | 53.02 | 6 |
| 10 | ATOM | 3787 | CD | GLN | B | 216 | 56.839 | 3.002 | 40.322 | 1.00 | 54.94 | 6 |
| | ATOM | 3788 | OE1 | GLN | B | 216 | 55.736 | 2.658 | 39.896 | 1.00 | 57.54 | 8 |
| | ATOM | 3789 | NE2 | GLN | B | 216 | 57.710 | 2.210 | 40.927 | 1.00 | 55.50 | 7 |
| | ATOM | 3790 | N | ALA | B | 217 | 57.092 | 7.678 | 43.486 | 1.00 | 46.68 | 7 |
| | ATOM | 3791 | CA | ALA | B | 217 | 56.502 | 8.282 | 44.665 | 1.00 | 47.12 | 6 |
| 15 | ATOM | 3792 | C | ALA | B | 217 | 56.114 | 9.746 | 44.444 | 1.00 | 46.63 | 6 |
| | ATOM | 3793 | O | ALA | B | 217 | 55.403 | 10.274 | 45.308 | 1.00 | 47.81 | 8 |
| | ATOM | 3794 | CB | ALA | B | 217 | 57.460 | 8.177 | 45.853 | 1.00 | 46.15 | 6 |
| | ATOM | 3795 | N | GLY | B | 218 | 56.519 | 10.406 | 43.374 | 1.00 | 45.52 | 7 |
| | ATOM | 3796 | CA | GLY | B | 218 | 56.156 | 11.790 | 43.127 | 1.00 | 45.00 | 6 |
| 20 | ATOM | 3797 | C | GLY | B | 218 | 57.308 | 12.764 | 43.230 | 1.00 | 45.03 | 6 |
| | ATOM | 3798 | O | GLY | B | 218 | 57.199 | 13.970 | 42.964 | 1.00 | 45.86 | 8 |
| | ATOM | 3799 | N | GLU | B | 219 | 58.491 | 12.255 | 43.605 | 1.00 | 43.84 | 7 |
| | ATOM | 3800 | CA | GLU | B | 219 | 59.664 | 13.121 | 43.708 | 1.00 | 43.09 | 6 |
| | ATOM | 3801 | C | GLU | B | 219 | 60.052 | 13.746 | 42.388 | 1.00 | 40.95 | 6 |
| 25 | ATOM | 3802 | O | GLU | B | 219 | 60.141 | 13.088 | 41.333 | 1.00 | 39.42 | 8 |
| | ATOM | 3803 | CB | GLU | B | 219 | 60.804 | 12.270 | 44.287 | 1.00 | 45.88 | 6 |
| | ATOM | 3804 | CG | GLU | B | 219 | 61.238 | 12.787 | 45.633 | 1.00 | 50.50 | 6 |
| | ATOM | 3805 | CD | GLU | B | 219 | 62.401 | 12.048 | 46.269 | 1.00 | 52.33 | 6 |
| | ATOM | 3806 | OE1 | GLU | B | 219 | 62.065 | 11.125 | 47.052 | 1.00 | 54.16 | 8 |
| 30 | ATOM | 3807 | OE2 | GLU | B | 219 | 63.564 | 12.388 | 46.016 | 1.00 | 53.19 | 8 |
| | ATOM | 3808 | N | ARG | B | 220 | 60.247 | 15.065 | 42.373 | 1.00 | 38.26 | 7 |
| | ATOM | 3809 | CA | ARG | B | 220 | 60.572 | 15.785 | 41.151 | 1.00 | 38.87 | 6 |
| | ATOM | 3810 | C | ARG | B | 220 | 61.803 | 16.664 | 41.272 | 1.00 | 38.94 | 6 |
| | ATOM | 3811 | O | ARG | B | 220 | 62.119 | 17.358 | 40.305 | 1.00 | 39.85 | 8 |
| 35 | ATOM | 3812 | CB | ARG | B | 220 | 59.396 | 16.676 | 40.670 | 1.00 | 39.03 | 6 |
| | ATOM | 3813 | CG | ARG | B | 220 | 58.187 | 15.871 | 40.179 | 1.00 | 39.62 | 6 |
| | ATOM | 3814 | CD | ARG | B | 220 | 58.562 | 15.016 | 38.972 | 1.00 | 39.07 | 6 |
| | ATOM | 3815 | NE | ARG | B | 220 | 57.490 | 14.110 | 38.632 | 1.00 | 39.25 | 7 |
| | ATOM | 3816 | CZ | ARG | B | 220 | 57.184 | 12.886 | 39.019 | 1.00 | 39.75 | 6 |
| 40 | ATOM | 3817 | NH1 | ARG | B | 220 | 57.946 | 12.211 | 39.893 | 1.00 | 39.07 | 7 |
| | ATOM | 3818 | NH2 | ARG | B | 220 | 56.073 | 12.331 | 38.529 | 1.00 | 38.25 | 7 |
| | ATOM | 3819 | N | ASP | B | 221 | 62.564 | 16.577 | 42.361 | 1.00 | 38.00 | 7 |
| | ATOM | 3820 | CA | ASP | B | 221 | 63.792 | 17.372 | 42.433 | 1.00 | 38.21 | 6 |
| | ATOM | 3821 | C | ASP | B | 221 | 64.911 | 16.557 | 41.791 | 1.00 | 36.88 | 6 |
| 45 | ATOM | 3822 | O | ASP | B | 221 | 65.691 | 15.899 | 42.474 | 1.00 | 36.84 | 8 |
| | ATOM | 3823 | CB | ASP | B | 221 | 64.146 | 17.760 | 43.866 | 1.00 | 40.08 | 6 |
| | ATOM | 3824 | CG | ASP | B | 221 | 65.276 | 18.775 | 43.867 | 1.00 | 40.98 | 6 |
| | ATOM | 3825 | OD1 | ASP | B | 221 | 66.189 | 18.865 | 43.017 | 1.00 | 40.33 | 8 |
| | ATOM | 3826 | OD2 | ASP | B | 221 | 65.237 | 19.583 | 44.824 | 1.00 | 45.27 | 8 |
| 50 | ATOM | 3827 | N | LEU | B | 222 | 64.940 | 16.559 | 40.472 | 1.00 | 36.51 | 7 |
| | ATOM | 3828 | CA | LEU | B | 222 | 65.839 | 15.703 | 39.697 | 1.00 | 35.37 | 6 |
| | ATOM | 3829 | C | LEU | B | 222 | 67.312 | 15.852 | 40.004 | 1.00 | 34.02 | 6 |
| | ATOM | 3830 | O | LEU | B | 222 | 68.053 | 14.855 | 40.041 | 1.00 | 31.24 | 8 |
| | ATOM | 3831 | CB | LEU | B | 222 | 65.575 | 15.983 | 38.203 | 1.00 | 35.83 | 6 |
| 55 | ATOM | 3832 | CG | LEU | B | 222 | 64.144 | 15.686 | 37.720 | 1.00 | 38.11 | 6 |
| | ATOM | 3833 | CD1 | LEU | B | 222 | 64.187 | 15.314 | 36.239 | 1.00 | 38.86 | 6 |
| | ATOM | 3834 | CD2 | LEU | B | 222 | 63.430 | 14.608 | 38.526 | 1.00 | 36.91 | 6 |
| | ATOM | 3835 | N | ASP | B | 223 | 67.763 | 17.101 | 40.153 | 1.00 | 33.49 | 7 |
| | ATOM | 3836 | CA | ASP | B | 223 | 69.154 | 17.349 | 40.442 | 1.00 | 33.63 | 6 |
| 60 | ATOM | 3837 | C | ASP | B | 223 | 69.524 | 16.656 | 41.751 | 1.00 | 31.73 | 6 |
| | ATOM | 3838 | O | ASP | B | 223 | 70.620 | 16.132 | 41.870 | 1.00 | 31.34 | 8 |
| | ATOM | 3839 | CB | ASP | B | 223 | 69.494 | 18.827 | 40.653 | 1.00 | 34.33 | 6 |
| | ATOM | 3840 | N | GLU | B | 224 | 68.635 | 16.790 | 42.733 | 1.00 | 31.71 | 7 |
| | ATOM | 3841 | CA | GLU | B | 224 | 68.909 | 16.161 | 44.035 | 1.00 | 31.51 | 6 |
| 65 | ATOM | 3842 | C | GLU | B | 224 | 68.836 | 14.656 | 43.974 | 1.00 | 29.02 | 6 |
| | ATOM | 3843 | O | GLU | B | 224 | 69.667 | 13.945 | 44.502 | 1.00 | 28.00 | 8 |
| | ATOM | 3844 | CB | GLU | B | 224 | 67.907 | 16.696 | 45.089 | 1.00 | 34.56 | 6 |
| | ATOM | 3845 | CG | GLU | B | 224 | 68.123 | 16.063 | 46.454 | 1.00 | 37.72 | 6 |
| | ATOM | 3846 | CD | GLU | B | 224 | 69.389 | 16.542 | 47.140 | 1.00 | 42.79 | 6 |
| 70 | ATOM | 3847 | OE1 | GLU | B | 224 | 70.120 | 17.403 | 46.574 | 1.00 | 43.28 | 8 |
| | ATOM | 3848 | OE2 | GLU | B | 224 | 69.660 | 16.051 | 48.273 | 1.00 | 43.45 | 8 |
| | ATOM | 3849 | N | ILE | B | 225 | 67.863 | 14.079 | 43.231 | 1.00 | 27.24 | 7 |
| | ATOM | 3850 | CA | ILE | B | 225 | 67.835 | 12.642 | 43.056 | 1.00 | 26.19 | 6 |
| | ATOM | 3851 | C | ILE | B | 225 | 69.109 | 12.145 | 42.417 | 1.00 | 25.15 | 6 |
| | ATOM | 3852 | O | ILE | B | 225 | 69.651 | 11.121 | 42.828 | 1.00 | 26.25 | 8 |

-89-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3853 | CB | ILE | B | 225 | 66.632 | 12.214 | 42.152 | 1.00 | 28.29 | 6 |
| | ATOM | 3854 | CG1 | ILE | B | 225 | 65.340 | 12.494 | 42.878 | 1.00 | 29.03 | 6 |
| | ATOM | 3855 | CG2 | ILE | B | 225 | 66.803 | 10.740 | 41.776 | 1.00 | 25.65 | 6 |
| 5 | ATOM | 3856 | CD1 | ILE | B | 225 | 64.109 | 12.596 | 42.001 | 1.00 | 31.93 | 6 |
| | ATOM | 3857 | N | ILE | B | 226 | 69.578 | 12.801 | 41.373 | 1.00 | 26.43 | 7 |
| | ATOM | 3858 | CA | ILE | B | 226 | 70.786 | 12.406 | 40.641 | 1.00 | 25.84 | 6 |
| | ATOM | 3859 | C | ILE | B | 226 | 72.040 | 12.551 | 41.500 | 1.00 | 27.10 | 6 |
| | ATOM | 3860 | O | ILE | B | 226 | 72.923 | 11.716 | 41.451 | 1.00 | 24.94 | 8 |
| 10 | ATOM | 3861 | CB | ILE | B | 226 | 70.923 | 13.170 | 39.304 | 1.00 | 27.17 | 6 |
| | ATOM | 3862 | CG1 | ILE | B | 226 | 69.753 | 12.662 | 38.429 | 1.00 | 27.18 | 6 |
| | ATOM | 3863 | CG2 | ILE | B | 226 | 72.280 | 12.981 | 38.632 | 1.00 | 27.48 | 6 |
| | ATOM | 3864 | CD1 | ILE | B | 226 | 69.562 | 13.504 | 37.159 | 1.00 | 27.31 | 6 |
| | ATOM | 3865 | N | THR | B | 227 | 72.095 | 13.642 | 42.283 | 1.00 | 25.81 | 7 |
| 15 | ATOM | 3866 | CA | THR | B | 227 | 73.300 | 13.811 | 43.112 | 1.00 | 25.80 | 6 |
| | ATOM | 3867 | C | THR | B | 227 | 73.368 | 12.725 | 44.157 | 1.00 | 24.81 | 6 |
| | ATOM | 3868 | O | THR | B | 227 | 74.457 | 12.188 | 44.484 | 1.00 | 23.72 | 8 |
| | ATOM | 3869 | CB | THR | B | 227 | 73.230 | 15.226 | 43.714 | 1.00 | 25.87 | 6 |
| | ATOM | 3870 | OG1 | THR | B | 227 | 73.461 | 16.226 | 42.719 | 1.00 | 27.10 | 8 |
| 20 | ATOM | 3871 | CG2 | THR | B | 227 | 74.317 | 15.419 | 44.776 | 1.00 | 30.13 | 6 |
| | ATOM | 3872 | N | ILE | B | 228 | 72.202 | 12.447 | 44.753 | 1.00 | 21.50 | 7 |
| | ATOM | 3873 | CA | ILE | B | 228 | 72.230 | 11.384 | 45.756 | 1.00 | 21.63 | 6 |
| | ATOM | 3874 | C | ILE | B | 228 | 72.645 | 10.046 | 45.160 | 1.00 | 23.87 | 6 |
| | ATOM | 3875 | O | ILE | B | 228 | 73.410 | 9.242 | 45.679 | 1.00 | 22.19 | 8 |
| 25 | ATOM | 3876 | CB | ILE | B | 228 | 70.892 | 11.236 | 46.481 | 1.00 | 21.84 | 6 |
| | ATOM | 3877 | CG1 | ILE | B | 228 | 70.746 | 12.501 | 47.397 | 1.00 | 24.08 | 6 |
| | ATOM | 3878 | CG2 | ILE | B | 228 | 70.762 | 9.964 | 47.278 | 1.00 | 22.76 | 6 |
| | ATOM | 3879 | CD1 | ILE | B | 228 | 69.295 | 12.583 | 47.901 | 1.00 | 26.19 | 6 |
| | ATOM | 3880 | N | ALA | B | 229 | 72.035 | 9.747 | 43.962 | 1.00 | 23.45 | 7 |
| 30 | ATOM | 3881 | CA | ALA | B | 229 | 72.386 | 8.510 | 43.308 | 1.00 | 24.32 | 6 |
| | ATOM | 3882 | C | ALA | B | 229 | 73.835 | 8.419 | 42.943 | 1.00 | 21.10 | 6 |
| | ATOM | 3883 | O | ALA | B | 229 | 74.403 | 7.325 | 43.107 | 1.00 | 23.01 | 8 |
| | ATOM | 3884 | CB | ALA | B | 229 | 71.481 | 8.404 | 42.050 | 1.00 | 22.78 | 6 |
| | ATOM | 3885 | N | GLY | B | 230 | 74.533 | 9.496 | 42.596 | 1.00 | 22.98 | 7 |
| 35 | ATOM | 3886 | CA | GLY | B | 230 | 75.940 | 9.540 | 42.325 | 1.00 | 25.69 | 6 |
| | ATOM | 3887 | C | GLY | B | 230 | 76.731 | 9.266 | 43.636 | 1.00 | 25.98 | 6 |
| | ATOM | 3888 | O | GLY | B | 230 | 77.669 | 8.455 | 43.656 | 1.00 | 23.67 | 8 |
| | ATOM | 3889 | N | GLN | B | 231 | 76.233 | 9.789 | 44.748 | 1.00 | 25.92 | 7 |
| | ATOM | 3890 | CA | GLN | B | 231 | 76.907 | 9.478 | 46.035 | 1.00 | 27.99 | 6 |
| 40 | ATOM | 3891 | C | GLN | B | 231 | 76.700 | 8.048 | 46.427 | 1.00 | 26.47 | 6 |
| | ATOM | 3892 | O | GLN | B | 231 | 77.666 | 7.384 | 46.850 | 1.00 | 25.84 | 8 |
| | ATOM | 3893 | CB | GLN | B | 231 | 76.407 | 10.471 | 47.120 | 1.00 | 28.03 | 6 |
| | ATOM | 3894 | CG | GLN | B | 231 | 76.834 | 10.043 | 48.531 | 1.00 | 32.38 | 6 |
| | ATOM | 3895 | CD | GLN | B | 231 | 78.316 | 10.219 | 48.756 | 1.00 | 32.95 | 6 |
| 45 | ATOM | 3896 | OE1 | GLN | B | 231 | 79.045 | 10.701 | 47.905 | 1.00 | 33.95 | 8 |
| | ATOM | 3897 | NE2 | GLN | B | 231 | 78.780 | 9.786 | 49.922 | 1.00 | 36.62 | 7 |
| | ATOM | 3898 | N | GLU | B | 232 | 75.516 | 7.434 | 46.178 | 1.00 | 26.86 | 7 |
| | ATOM | 3899 | CA | GLU | B | 232 | 75.285 | 6.024 | 46.475 | 1.00 | 25.40 | 6 |
| | ATOM | 3900 | C | GLU | B | 232 | 76.193 | 5.139 | 45.605 | 1.00 | 27.57 | 6 |
| 50 | ATOM | 3901 | O | GLU | B | 232 | 76.802 | 4.178 | 46.110 | 1.00 | 28.11 | 8 |
| | ATOM | 3902 | CB | GLU | B | 232 | 73.827 | 5.559 | 46.287 | 1.00 | 27.07 | 6 |
| | ATOM | 3903 | CG | GLU | B | 232 | 72.820 | 6.282 | 47.171 | 1.00 | 30.63 | 6 |
| | ATOM | 3904 | CD | GLU | B | 232 | 71.375 | 5.946 | 46.930 | 1.00 | 34.51 | 6 |
| | ATOM | 3905 | OE1 | GLU | B | 232 | 71.033 | 5.379 | 45.860 | 1.00 | 37.23 | 8 |
| 55 | ATOM | 3906 | OE2 | GLU | B | 232 | 70.510 | 6.232 | 47.794 | 1.00 | 35.98 | 8 |
| | ATOM | 3907 | N | LEU | B | 233 | 76.346 | 5.489 | 44.313 | 1.00 | 26.60 | 7 |
| | ATOM | 3908 | CA | LEU | B | 233 | 77.272 | 4.700 | 43.490 | 1.00 | 26.30 | 6 |
| | ATOM | 3909 | C | LEU | B | 233 | 78.710 | 4.784 | 44.024 | 1.00 | 28.83 | 6 |
| | ATOM | 3910 | O | LEU | B | 233 | 79.402 | 3.781 | 44.040 | 1.00 | 28.19 | 8 |
| 60 | ATOM | 3911 | CB | LEU | B | 233 | 77.171 | 5.171 | 42.025 | 1.00 | 27.72 | 6 |
| | ATOM | 3912 | CG | LEU | B | 233 | 75.816 | 4.809 | 41.372 | 1.00 | 26.70 | 6 |
| | ATOM | 3913 | CD1 | LEU | B | 233 | 75.511 | 5.576 | 40.104 | 1.00 | 27.51 | 6 |
| | ATOM | 3914 | CD2 | LEU | B | 233 | 75.819 | 3.312 | 41.048 | 1.00 | 28.08 | 6 |
| | ATOM | 3915 | N | ASN | B | 234 | 79.166 | 6.006 | 44.330 | 1.00 | 31.21 | 7 |
| 65 | ATOM | 3916 | CA | ASN | B | 234 | 80.540 | 6.248 | 44.790 | 1.00 | 32.86 | 6 |
| | ATOM | 3917 | C | ASN | B | 234 | 80.761 | 5.404 | 46.020 | 1.00 | 32.80 | 6 |
| | ATOM | 3918 | O | ASN | B | 234 | 81.764 | 4.675 | 46.099 | 1.00 | 34.18 | 8 |
| | ATOM | 3919 | CB | ASN | B | 234 | 80.775 | 7.750 | 45.048 | 1.00 | 33.46 | 6 |
| | ATOM | 3920 | CG | ASN | B | 234 | 82.187 | 8.099 | 45.503 | 1.00 | 38.46 | 6 |
| | ATOM | 3921 | OD1 | ASN | B | 234 | 82.545 | 7.889 | 46.687 | 1.00 | 39.27 | 8 |
| 70 | ATOM | 3922 | ND2 | ASN | B | 234 | 83.042 | 8.646 | 44.636 | 1.00 | 38.37 | 7 |
| | ATOM | 3923 | N | GLU | B | 235 | 79.781 | 5.385 | 46.942 | 1.00 | 32.30 | 7 |
| | ATOM | 3924 | CA | GLU | B | 235 | 79.995 | 4.556 | 48.156 | 1.00 | 34.69 | 6 |
| | ATOM | 3925 | C | GLU | B | 235 | 80.036 | 3.082 | 47.880 | 1.00 | 35.00 | 6 |
| | ATOM | 3926 | O | GLU | B | 235 | 80.783 | 2.325 | 48.548 | 1.00 | 34.91 | 8 |

-90-

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 3927 | CB | GLU | B | 235 | 78.927 | 4.941 | 49.210 | 1.00 | 35.01 | 6 |
| | ATOM | 3928 | N | LYS | B | 236 | 79.431 | 2.541 | 46.819 | 1.00 | 32.85 | 7 |
| | ATOM | 3929 | CA | LYS | B | 236 | 79.476 | 1.161 | 46.438 | 1.00 | 32.12 | 6 |
| 5 | ATOM | 3930 | C | LYS | B | 236 | 80.733 | 0.795 | 45.662 | 1.00 | 31.23 | 6 |
| | ATOM | 3931 | O | LYS | B | 236 | 81.027 | -0.387 | 45.442 | 1.00 | 32.24 | 8 |
| | ATOM | 3932 | CB | LYS | B | 236 | 78.257 | 0.838 | 45.530 | 1.00 | 31.56 | 6 |
| | ATOM | 3933 | CG | LYS | B | 236 | 76.968 | 0.739 | 46.321 | 1.00 | 33.04 | 6 |
| | ATOM | 3934 | CD | LYS | B | 236 | 75.825 | 0.425 | 45.347 | 1.00 | 34.58 | 6 |
| 10 | ATOM | 3935 | CE | LYS | B | 236 | 74.486 | 0.657 | 46.017 | 1.00 | 38.11 | 6 |
| | ATOM | 3936 | NZ | LYS | B | 236 | 74.152 | -0.406 | 47.008 | 1.00 | 41.00 | 7 |
| | ATOM | 3937 | N | GLY | B | 237 | 81.463 | 1.790 | 45.196 | 1.00 | 31.15 | 7 |
| | ATOM | 3938 | CA | GLY | B | 237 | 82.701 | 1.595 | 44.467 | 1.00 | 32.69 | 6 |
| | ATOM | 3939 | C | GLY | B | 237 | 82.728 | 2.025 | 43.030 | 1.00 | 33.87 | 6 |
| 15 | ATOM | 3940 | O | GLY | B | 237 | 83.730 | 1.798 | 42.345 | 1.00 | 36.00 | 8 |
| | ATOM | 3941 | N | PHE | B | 238 | 81.635 | 2.625 | 42.522 | 1.00 | 30.77 | 7 |
| | ATOM | 3942 | CA | PHE | B | 238 | 81.579 | 3.079 | 41.154 | 1.00 | 31.26 | 6 |
| | ATOM | 3943 | C | PHE | B | 238 | 82.111 | 4.488 | 41.041 | 1.00 | 32.04 | 6 |
| | ATOM | 3944 | O | PHE | B | 238 | 82.216 | 5.186 | 42.067 | 1.00 | 32.73 | 8 |
| 20 | ATOM | 3945 | CB | PHE | B | 238 | 80.125 | 3.016 | 40.628 | 1.00 | 31.33 | 6 |
| | ATOM | 3946 | CG | PHE | B | 238 | 79.481 | 1.668 | 40.628 | 1.00 | 29.12 | 6 |
| | ATOM | 3947 | CD1 | PHE | B | 238 | 78.935 | 1.079 | 41.736 | 1.00 | 29.70 | 6 |
| | ATOM | 3948 | CD2 | PHE | B | 238 | 79.401 | 0.975 | 39.390 | 1.00 | 29.67 | 6 |
| | ATOM | 3949 | CE1 | PHE | B | 238 | 78.325 | -0.181 | 41.661 | 1.00 | 30.02 | 6 |
| 25 | ATOM | 3950 | CE2 | PHE | B | 238 | 78.805 | -0.265 | 39.328 | 1.00 | 28.39 | 6 |
| | ATOM | 3951 | CZ | PHE | B | 238 | 78.268 | -0.858 | 40.457 | 1.00 | 29.71 | 6 |
| | ATOM | 3952 | N | ARG | B | 239 | 82.539 | 4.918 | 39.876 | 1.00 | 32.94 | 7 |
| | ATOM | 3953 | CA | ARG | B | 239 | 83.050 | 6.269 | 39.716 | 1.00 | 35.90 | 6 |
| | ATOM | 3954 | C | ARG | B | 239 | 82.426 | 6.906 | 38.487 | 1.00 | 38.53 | 6 |
| 30 | ATOM | 3955 | O | ARG | B | 239 | 81.735 | 6.244 | 37.694 | 1.00 | 38.62 | 8 |
| | ATOM | 3956 | CB | ARG | B | 239 | 84.581 | 6.280 | 39.597 | 1.00 | 35.70 | 6 |
| | ATOM | 3957 | CG | ARG | B | 239 | 85.340 | 5.894 | 40.856 | 1.00 | 36.08 | 6 |
| | ATOM | 3958 | CD | ARG | B | 239 | 85.108 | 6.926 | 41.956 | 1.00 | 35.58 | 6 |
| | ATOM | 3959 | NE | ARG | B | 239 | 85.710 | 6.612 | 43.215 | 1.00 | 36.21 | 7 |
| 35 | ATOM | 3960 | CZ | ARG | B | 239 | 85.280 | 5.815 | 44.190 | 1.00 | 37.41 | 6 |
| | ATOM | 3961 | NH1 | ARG | B | 239 | 84.113 | 5.159 | 44.129 | 1.00 | 35.39 | 7 |
| | ATOM | 3962 | NH2 | ARG | B | 239 | 86.015 | 5.707 | 45.288 | 1.00 | 35.70 | 7 |
| | ATOM | 3963 | N | ALA | B | 240 | 82.667 | 8.199 | 38.339 | 1.00 | 38.40 | 7 |
| | ATOM | 3964 | CA | ALA | B | 240 | 82.310 | 8.977 | 37.152 | 1.00 | 39.45 | 6 |
| 40 | ATOM | 3965 | C | ALA | B | 240 | 80.954 | 8.630 | 36.553 | 1.00 | 39.96 | 6 |
| | ATOM | 3966 | O | ALA | B | 240 | 80.846 | 8.388 | 35.348 | 1.00 | 41.59 | 8 |
| | ATOM | 3967 | CB | ALA | B | 240 | 83.408 | 8.761 | 36.103 | 1.00 | 39.64 | 6 |
| | ATOM | 3968 | N | ASP | B | 241 | 79.899 | 8.687 | 37.369 | 1.00 | 39.86 | 7 |
| | ATOM | 3969 | CA | ASP | B | 241 | 78.567 | 8.382 | 36.881 | 1.00 | 37.91 | 6 |
| 45 | ATOM | 3970 | C | ASP | B | 241 | 78.087 | 9.495 | 35.947 | 1.00 | 39.44 | 6 |
| | ATOM | 3971 | O | ASP | B | 241 | 78.464 | 10.658 | 36.063 | 1.00 | 38.78 | 8 |
| | ATOM | 3972 | CB | ASP | B | 241 | 77.554 | 8.232 | 38.028 | 1.00 | 39.68 | 6 |
| | ATOM | 3973 | CG | ASP | B | 241 | 77.464 | 9.573 | 38.758 | 1.00 | 42.34 | 6 |
| | ATOM | 3974 | OD1 | ASP | B | 241 | 76.577 | 10.419 | 38.447 | 1.00 | 44.14 | 8 |
| 50 | ATOM | 3975 | OD2 | ASP | B | 241 | 78.353 | 9.828 | 39.610 | 1.00 | 41.04 | 8 |
| | ATOM | 3976 | N | ASP | B | 242 | 77.220 | 9.122 | 35.028 | 1.00 | 36.17 | 7 |
| | ATOM | 3977 | CA | ASP | B | 242 | 76.543 | 10.050 | 34.122 | 1.00 | 36.78 | 6 |
| | ATOM | 3978 | C | ASP | B | 242 | 75.102 | 9.548 | 34.108 | 1.00 | 32.97 | 6 |
| | ATOM | 3979 | O | ASP | B | 242 | 74.890 | 8.412 | 33.654 | 1.00 | 32.78 | 8 |
| 55 | ATOM | 3980 | CB | ASP | B | 242 | 77.160 | 10.107 | 32.755 | 1.00 | 41.35 | 6 |
| | ATOM | 3981 | CG | ASP | B | 242 | 76.317 | 10.792 | 31.704 | 1.00 | 46.81 | 6 |
| | ATOM | 3982 | OD1 | ASP | B | 242 | 76.414 | 10.318 | 30.543 | 1.00 | 50.98 | 8 |
| | ATOM | 3983 | OD2 | ASP | B | 242 | 75.539 | 11.741 | 31.944 | 1.00 | 49.34 | 8 |
| | ATOM | 3984 | N | ILE | B | 243 | 74.204 | 10.301 | 34.710 | 1.00 | 29.36 | 7 |
| 60 | ATOM | 3985 | CA | ILE | B | 243 | 72.817 | 9.893 | 34.861 | 1.00 | 27.87 | 6 |
| | ATOM | 3986 | C | ILE | B | 243 | 71.890 | 10.907 | 34.213 | 1.00 | 28.93 | 6 |
| | ATOM | 3987 | O | ILE | B | 243 | 71.986 | 12.098 | 34.489 | 1.00 | 28.18 | 8 |
| | ATOM | 3988 | CB | ILE | B | 243 | 72.407 | 9.746 | 36.339 | 1.00 | 28.09 | 6 |
| | ATOM | 3989 | CG1 | ILE | B | 243 | 73.240 | 8.680 | 37.065 | 1.00 | 28.98 | 6 |
| 65 | ATOM | 3990 | CG2 | ILE | B | 243 | 70.934 | 9.373 | 36.477 | 1.00 | 26.56 | 6 |
| | ATOM | 3991 | CD1 | ILE | B | 243 | 73.044 | 8.655 | 38.575 | 1.00 | 28.71 | 6 |
| | ATOM | 3992 | N | GLN | B | 244 | 70.912 | 10.442 | 33.437 | 1.00 | 27.35 | 7 |
| | ATOM | 3993 | CA | GLN | B | 244 | 69.944 | 11.390 | 32.837 | 1.00 | 29.56 | 6 |
| | ATOM | 3994 | C | GLN | B | 244 | 68.550 | 10.906 | 33.126 | 1.00 | 28.63 | 6 |
| 70 | ATOM | 3995 | O | GLN | B | 244 | 68.328 | 9.670 | 33.170 | 1.00 | 28.44 | 8 |
| | ATOM | 3996 | CB | GLN | B | 244 | 70.154 | 11.546 | 31.342 | 1.00 | 32.37 | 6 |
| | ATOM | 3997 | CG | GLN | B | 244 | 71.494 | 11.871 | 30.754 | 1.00 | 33.10 | 6 |
| | ATOM | 3998 | N | ILE | B | 245 | 67.580 | 11.792 | 33.287 | 1.00 | 28.47 | 7 |
| | ATOM | 3999 | CA | ILE | B | 245 | 66.194 | 11.454 | 33.560 | 1.00 | 27.98 | 6 |
| | ATOM | 4000 | C | ILE | B | 245 | 65.367 | 12.295 | 32.544 | 1.00 | 29.53 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 4001 | O | ILE | B | 245 | 65.647 | 13.473 | 32.427 | 1.00 | 28.72 | 8 |
| | ATOM | 4002 | CB | ILE | B | 245 | 65.647 | 11.723 | 34.955 | 1.00 | 30.08 | 6 |
| | ATOM | 4003 | CG1 | ILE | B | 245 | 66.275 | 10.837 | 36.048 | 1.00 | 31.65 | 6 |
| 5 | ATOM | 4004 | CG2 | ILE | B | 245 | 64.136 | 11.475 | 34.988 | 1.00 | 30.80 | 6 |
| | ATOM | 4005 | CD1 | ILE | B | 245 | 65.994 | 11.415 | 37.433 | 1.00 | 33.41 | 6 |
| | ATOM | 4006 | N | ARG | B | 246 | 64.608 | 11.578 | 31.703 | 1.00 | 28.63 | 7 |
| | ATOM | 4007 | CA | ARG | B | 246 | 63.903 | 12.319 | 30.635 | 1.00 | 29.40 | 6 |
| | ATOM | 4008 | C | ARG | B | 246 | 62.475 | 11.841 | 30.597 | 1.00 | 29.33 | 6 |
| | ATOM | 4009 | O | ARG | B | 246 | 62.198 | 10.775 | 31.136 | 1.00 | 29.29 | 8 |
| 10 | ATOM | 4010 | CB | ARG | B | 246 | 64.481 | 12.084 | 29.252 | 1.00 | 33.51 | 6 |
| | ATOM | 4011 | CG | ARG | B | 246 | 65.896 | 12.479 | 29.026 | 1.00 | 37.29 | 6 |
| | ATOM | 4012 | CD | ARG | B | 246 | 66.517 | 12.212 | 27.672 | 1.00 | 42.16 | 6 |
| | ATOM | 4013 | NE | ARG | B | 246 | 67.527 | 13.251 | 27.472 | 1.00 | 47.11 | 7 |
| | ATOM | 4014 | CZ | ARG | B | 246 | 68.770 | 13.142 | 27.056 | 1.00 | 50.44 | 6 |
| 15 | ATOM | 4015 | NH1 | ARG | B | 246 | 69.318 | 11.970 | 26.737 | 1.00 | 53.10 | 7 |
| | ATOM | 4016 | NH2 | ARG | B | 246 | 69.502 | 14.252 | 26.974 | 1.00 | 51.57 | 7 |
| | ATOM | 4017 | N | ASP | B | 247 | 61.544 | 12.634 | 30.039 | 1.00 | 28.70 | 7 |
| | ATOM | 4018 | CA | ASP | B | 247 | 60.185 | 12.189 | 29.792 | 1.00 | 29.87 | 6 |
| 20 | ATOM | 4019 | C | ASP | B | 247 | 60.289 | 11.146 | 28.656 | 1.00 | 25.96 | 6 |
| | ATOM | 4020 | O | ASP | B | 247 | 60.989 | 11.431 | 27.671 | 1.00 | 27.47 | 8 |
| | ATOM | 4021 | CB | ASP | B | 247 | 59.303 | 13.349 | 29.389 | 1.00 | 31.15 | 6 |
| | ATOM | 4022 | CG | ASP | B | 247 | 57.894 | 13.014 | 28.997 | 1.00 | 33.47 | 6 |
| | ATOM | 4023 | OD1 | ASP | B | 247 | 57.667 | 12.084 | 28.184 | 1.00 | 32.45 | 8 |
| 25 | ATOM | 4024 | OD2 | ASP | B | 247 | 56.982 | 13.703 | 29.524 | 1.00 | 33.36 | 8 |
| | ATOM | 4025 | N | ALA | B | 248 | 59.759 | 9.981 | 28.873 | 1.00 | 27.20 | 7 |
| | ATOM | 4026 | CA | ALA | B | 248 | 59.987 | 8.893 | 27.906 | 1.00 | 28.58 | 6 |
| | ATOM | 4027 | C | ALA | B | 248 | 59.141 | 9.055 | 26.643 | 1.00 | 29.88 | 6 |
| | ATOM | 4028 | O | ALA | B | 248 | 59.444 | 8.315 | 25.702 | 1.00 | 29.99 | 8 |
| 30 | ATOM | 4029 | CB | ALA | B | 248 | 59.652 | 7.572 | 28.566 | 1.00 | 28.03 | 6 |
| | ATOM | 4030 | N | ASP | B | 249 | 58.121 | 9.877 | 26.724 | 1.00 | 28.08 | 7 |
| | ATOM | 4031 | CA | ASP | B | 249 | 57.293 | 10.116 | 25.513 | 1.00 | 30.80 | 6 |
| | ATOM | 4032 | C | ASP | B | 249 | 57.764 | 11.262 | 24.667 | 1.00 | 29.85 | 6 |
| | ATOM | 4033 | O | ASP | B | 249 | 57.690 | 11.217 | 23.402 | 1.00 | 30.23 | 8 |
| 35 | ATOM | 4034 | CB | ASP | B | 249 | 55.853 | 10.392 | 25.955 | 1.00 | 32.78 | 6 |
| | ATOM | 4035 | CG | ASP | B | 249 | 55.226 | 9.204 | 26.623 | 1.00 | 37.46 | 6 |
| | ATOM | 4036 | OD1 | ASP | B | 249 | 55.538 | 8.084 | 26.164 | 1.00 | 39.14 | 8 |
| | ATOM | 4037 | OD2 | ASP | B | 249 | 54.448 | 9.329 | 27.595 | 1.00 | 39.72 | 8 |
| | ATOM | 4038 | N | THR | B | 250 | 58.264 | 12.361 | 25.283 | 1.00 | 26.32 | 7 |
| 40 | ATOM | 4039 | CA | THR | B | 250 | 58.710 | 13.526 | 24.523 | 1.00 | 27.61 | 6 |
| | ATOM | 4040 | C | THR | B | 250 | 60.191 | 13.683 | 24.413 | 1.00 | 26.93 | 6 |
| | ATOM | 4041 | O | THR | B | 250 | 60.785 | 14.328 | 23.570 | 1.00 | 28.19 | 8 |
| | ATOM | 4042 | CB | THR | B | 250 | 58.162 | 14.831 | 25.186 | 1.00 | 30.35 | 6 |
| | ATOM | 4043 | OG1 | THR | B | 250 | 58.797 | 14.978 | 26.457 | 1.00 | 31.06 | 8 |
| 45 | ATOM | 4044 | CG2 | THR | B | 250 | 56.677 | 14.760 | 25.380 | 1.00 | 32.40 | 6 |
| | ATOM | 4045 | N | LEU | B | 251 | 60.891 | 12.958 | 25.324 | 1.00 | 27.41 | 7 |
| | ATOM | 4046 | CA | LEU | B | 251 | 62.336 | 12.857 | 25.461 | 1.00 | 30.17 | 6 |
| | ATOM | 4047 | C | LEU | B | 251 | 62.928 | 14.204 | 25.968 | 1.00 | 31.32 | 6 |
| | ATOM | 4048 | O | LEU | B | 251 | 64.110 | 14.434 | 25.775 | 1.00 | 33.84 | 8 |
| 50 | ATOM | 4049 | CB | LEU | B | 251 | 63.096 | 12.483 | 24.205 | 1.00 | 30.53 | 6 |
| | ATOM | 4050 | CG | LEU | B | 251 | 62.568 | 11.151 | 23.560 | 1.00 | 30.23 | 6 |
| | ATOM | 4051 | CD1 | LEU | B | 251 | 63.382 | 10.891 | 22.307 | 1.00 | 31.95 | 6 |
| | ATOM | 4052 | CD2 | LEU | B | 251 | 62.575 | 10.004 | 24.541 | 1.00 | 30.44 | 6 |
| | ATOM | 4053 | N | LEU | B | 252 | 62.054 | 15.017 | 26.483 | 1.00 | 33.09 | 7 |
| 55 | ATOM | 4054 | CA | LEU | B | 252 | 62.441 | 16.323 | 27.015 | 1.00 | 34.68 | 6 |
| | ATOM | 4055 | C | LEU | B | 252 | 62.530 | 16.162 | 28.519 | 1.00 | 35.10 | 6 |
| | ATOM | 4056 | O | LEU | B | 252 | 62.436 | 15.037 | 29.003 | 1.00 | 30.04 | 8 |
| | ATOM | 4057 | CB | LEU | B | 252 | 61.439 | 17.401 | 26.633 | 1.00 | 35.48 | 6 |
| | ATOM | 4058 | CG | LEU | B | 252 | 61.476 | 17.664 | 25.106 | 1.00 | 38.16 | 6 |
| 60 | ATOM | 4059 | CD1 | LEU | B | 252 | 60.219 | 18.416 | 24.715 | 1.00 | 38.56 | 6 |
| | ATOM | 4060 | CD2 | LEU | B | 252 | 62.782 | 18.361 | 24.789 | 1.00 | 38.57 | 6 |
| | ATOM | 4061 | N | GLU | B | 253 | 62.625 | 17.316 | 29.217 | 1.00 | 36.82 | 7 |
| | ATOM | 4062 | CA | GLU | B | 253 | 62.731 | 17.220 | 30.668 | 1.00 | 39.59 | 6 |
| | ATOM | 4063 | C | GLU | B | 253 | 61.417 | 16.777 | 31.259 | 1.00 | 39.50 | 6 |
| 65 | ATOM | 4064 | O | GLU | B | 253 | 60.403 | 17.042 | 30.591 | 1.00 | 40.91 | 8 |
| | ATOM | 4065 | CB | GLU | B | 253 | 63.103 | 18.586 | 31.274 | 1.00 | 42.93 | 6 |
| | ATOM | 4066 | CG | GLU | B | 253 | 64.342 | 19.202 | 30.643 | 1.00 | 48.27 | 6 |
| | ATOM | 4067 | CD | GLU | B | 253 | 65.560 | 18.356 | 30.999 | 1.00 | 51.88 | 6 |
| | ATOM | 4068 | OE1 | GLU | B | 253 | 65.758 | 18.143 | 32.226 | 1.00 | 54.42 | 8 |
| 70 | ATOM | 4069 | OE2 | GLU | B | 253 | 66.259 | 17.915 | 30.063 | 1.00 | 53.71 | 8 |
| | ATOM | 4070 | N | VAL | B | 254 | 61.405 | 16.130 | 32.403 | 1.00 | 39.00 | 7 |
| | ATOM | 4071 | CA | VAL | B | 254 | 60.167 | 15.751 | 33.062 | 1.00 | 40.35 | 6 |
| | ATOM | 4072 | C | VAL | B | 254 | 59.384 | 16.991 | 33.488 | 1.00 | 43.05 | 6 |
| | ATOM | 4073 | O | VAL | B | 254 | 59.955 | 17.997 | 33.903 | 1.00 | 42.79 | 8 |
| | ATOM | 4074 | CB | VAL | B | 254 | 60.425 | 14.856 | 34.285 | 1.00 | 39.32 | 6 |

-92-

| | | | | | | | | | | | | |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 4075 | CG1 | VAL | B | 254 | 59.162 | 14.614 | 35.088 | 1.00 | 37.70 | 6 |
| | ATOM | 4076 | CG2 | VAL | B | 254 | 61.054 | 13.553 | 33.783 | 1.00 | 38.29 | 6 |
| | ATOM | 4077 | N | SER | B | 255 | 58.070 | 16.937 | 33.293 | 1.00 | 46.50 | 7 |
| 5 | ATOM | 4078 | CA | SER | B | 255 | 57.178 | 18.041 | 33.641 | 1.00 | 47.57 | 6 |
| | ATOM | 4079 | C | SER | B | 255 | 56.027 | 17.520 | 34.498 | 1.00 | 48.72 | 6 |
| | ATOM | 4080 | O | SER | B | 255 | 56.063 | 16.436 | 35.062 | 1.00 | 49.33 | 8 |
| | ATOM | 4081 | CB | SER | B | 255 | 56.663 | 18.739 | 32.379 | 1.00 | 47.97 | 6 |
| | ATOM | 4082 | OG | SER | B | 255 | 55.566 | 18.022 | 31.814 | 1.00 | 50.04 | 8 |
| 10 | ATOM | 4083 | N | GLU | B | 256 | 54.990 | 18.358 | 34.593 | 1.00 | 48.58 | 7 |
| | ATOM | 4084 | CA | GLU | B | 256 | 53.787 | 18.010 | 35.346 | 1.00 | 49.19 | 6 |
| | ATOM | 4085 | C | GLU | B | 256 | 52.838 | 17.201 | 34.488 | 1.00 | 49.15 | 6 |
| | ATOM | 4086 | O | GLU | B | 256 | 51.953 | 16.493 | 34.969 | 1.00 | 50.39 | 8 |
| | ATOM | 4087 | CB | GLU | B | 256 | 53.154 | 19.321 | 35.844 | 1.00 | 49.68 | 6 |
| 15 | ATOM | 4088 | N | THR | B | 257 | 53.078 | 17.241 | 33.177 | 1.00 | 48.71 | 7 |
| | ATOM | 4089 | CA | THR | B | 257 | 52.306 | 16.471 | 32.211 | 1.00 | 49.54 | 6 |
| | ATOM | 4090 | C | THR | B | 257 | 52.962 | 15.121 | 31.914 | 1.00 | 48.26 | 6 |
| | ATOM | 4091 | O | THR | B | 257 | 52.333 | 14.259 | 31.285 | 1.00 | 48.37 | 8 |
| | ATOM | 4092 | CB | THR | B | 257 | 52.146 | 17.265 | 30.913 | 1.00 | 50.65 | 6 |
| 20 | ATOM | 4093 | OG1 | THR | B | 257 | 53.430 | 17.717 | 30.454 | 1.00 | 52.73 | 8 |
| | ATOM | 4094 | CG2 | THR | B | 257 | 51.277 | 18.496 | 31.154 | 1.00 | 52.44 | 6 |
| | ATOM | 4095 | N | SER | B | 258 | 54.201 | 14.933 | 32.368 | 1.00 | 44.00 | 7 |
| | ATOM | 4096 | CA | SER | B | 258 | 54.923 | 13.690 | 32.124 | 1.00 | 43.02 | 6 |
| | ATOM | 4097 | C | SER | B | 258 | 54.197 | 12.470 | 32.665 | 1.00 | 41.05 | 6 |
| 25 | ATOM | 4098 | O | SER | B | 258 | 53.785 | 12.435 | 33.808 | 1.00 | 40.25 | 8 |
| | ATOM | 4099 | CB | SER | B | 258 | 56.315 | 13.710 | 32.765 | 1.00 | 39.95 | 6 |
| | ATOM | 4100 | OG | SER | B | 258 | 57.171 | 14.561 | 32.020 | 1.00 | 37.63 | 8 |
| | ATOM | 4101 | N | LYS | B | 259 | 54.041 | 11.453 | 31.819 | 1.00 | 40.55 | 7 |
| | ATOM | 4102 | CA | LYS | B | 259 | 53.347 | 10.253 | 32.275 | 1.00 | 40.93 | 6 |
| 30 | ATOM | 4103 | C | LYS | B | 259 | 54.339 | 9.094 | 32.390 | 1.00 | 38.96 | 6 |
| | ATOM | 4104 | O | LYS | B | 259 | 54.036 | 8.130 | 33.071 | 1.00 | 39.56 | 8 |
| | ATOM | 4105 | CB | LYS | B | 259 | 52.193 | 9.870 | 31.340 | 1.00 | 44.20 | 6 |
| | ATOM | 4106 | CG | LYS | B | 259 | 51.223 | 11.038 | 31.184 | 1.00 | 47.43 | 6 |
| | ATOM | 4107 | CD | LYS | B | 259 | 49.868 | 10.656 | 30.608 | 1.00 | 50.95 | 6 |
| 35 | ATOM | 4108 | CE | LYS | B | 259 | 48.814 | 11.646 | 31.143 | 1.00 | 52.15 | 6 |
| | ATOM | 4109 | NZ | LYS | B | 259 | 47.678 | 11.728 | 30.177 | 1.00 | 54.34 | 7 |
| | ATOM | 4110 | N | ARG | B | 260 | 55.446 | 9.187 | 31.695 | 1.00 | 38.03 | 7 |
| | ATOM | 4111 | CA | ARG | B | 260 | 56.469 | 8.146 | 31.706 | 1.00 | 36.81 | 6 |
| | ATOM | 4112 | C | ARG | B | 260 | 57.852 | 8.765 | 31.794 | 1.00 | 33.36 | 6 |
| 40 | ATOM | 4113 | O | ARG | B | 260 | 58.150 | 9.717 | 31.075 | 1.00 | 30.91 | 8 |
| | ATOM | 4114 | CB | ARG | B | 260 | 56.438 | 7.267 | 30.445 | 1.00 | 38.22 | 6 |
| | ATOM | 4115 | CG | ARG | B | 260 | 55.182 | 6.504 | 30.103 | 1.00 | 42.83 | 6 |
| | ATOM | 4116 | CD | ARG | B | 260 | 55.389 | 5.584 | 28.896 | 1.00 | 43.79 | 6 |
| | ATOM | 4117 | NE | ARG | B | 260 | 54.174 | 4.856 | 28.536 | 1.00 | 46.34 | 7 |
| 45 | ATOM | 4118 | N | ALA | B | 261 | 58.808 | 8.142 | 32.519 | 1.00 | 31.91 | 7 |
| | ATOM | 4119 | CA | ALA | B | 261 | 60.182 | 8.623 | 32.486 | 1.00 | 28.39 | 6 |
| | ATOM | 4120 | C | ALA | B | 261 | 61.176 | 7.524 | 32.106 | 1.00 | 25.89 | 6 |
| | ATOM | 4121 | O | ALA | B | 261 | 60.882 | 6.354 | 32.381 | 1.00 | 29.01 | 8 |
| | ATOM | 4122 | CB | ALA | B | 261 | 60.695 | 9.169 | 33.836 | 1.00 | 29.25 | 6 |
| 50 | ATOM | 4123 | N | VAL | B | 262 | 62.238 | 7.874 | 31.454 | 1.00 | 27.17 | 7 |
| | ATOM | 4124 | CA | VAL | B | 262 | 63.325 | 6.947 | 31.122 | 1.00 | 29.12 | 6 |
| | ATOM | 4125 | C | VAL | B | 262 | 64.544 | 7.432 | 31.944 | 1.00 | 28.50 | 6 |
| | ATOM | 4126 | O | VAL | B | 262 | 64.860 | 8.605 | 31.932 | 1.00 | 27.83 | 8 |
| | ATOM | 4127 | CB | VAL | B | 262 | 63.659 | 6.838 | 29.647 | 1.00 | 30.51 | 6 |
| 55 | ATOM | 4128 | CG1 | VAL | B | 262 | 63.902 | 8.231 | 29.043 | 1.00 | 30.91 | 6 |
| | ATOM | 4129 | CG2 | VAL | B | 262 | 64.881 | 5.958 | 29.356 | 1.00 | 30.63 | 6 |
| | ATOM | 4130 | N | ILE | B | 263 | 65.221 | 6.505 | 32.611 | 1.00 | 29.18 | 7 |
| | ATOM | 4131 | CA | ILE | B | 263 | 66.406 | 6.792 | 33.454 | 1.00 | 27.39 | 6 |
| | ATOM | 4132 | C | ILE | B | 263 | 67.590 | 6.119 | 32.790 | 1.00 | 25.94 | 6 |
| 60 | ATOM | 4133 | O | ILE | B | 263 | 67.437 | 4.906 | 32.507 | 1.00 | 25.04 | 8 |
| | ATOM | 4134 | CB | ILE | B | 263 | 66.243 | 6.278 | 34.881 | 1.00 | 29.45 | 6 |
| | ATOM | 4135 | CG1 | ILE | B | 263 | 64.898 | 6.687 | 35.497 | 1.00 | 29.18 | 6 |
| | ATOM | 4136 | CG2 | ILE | B | 263 | 67.369 | 6.819 | 35.758 | 1.00 | 29.13 | 6 |
| | ATOM | 4137 | CD1 | ILE | B | 263 | 64.395 | 5.672 | 36.508 | 1.00 | 32.09 | 6 |
| 65 | ATOM | 4138 | N | LEU | B | 264 | 68.626 | 6.784 | 32.377 | 1.00 | 25.66 | 7 |
| | ATOM | 4139 | CA | LEU | B | 264 | 69.795 | 6.289 | 31.701 | 1.00 | 27.04 | 6 |
| | ATOM | 4140 | C | LEU | B | 264 | 70.978 | 6.430 | 32.666 | 1.00 | 29.07 | 6 |
| | ATOM | 4141 | O | LEU | B | 264 | 71.152 | 7.574 | 33.143 | 1.00 | 29.50 | 8 |
| | ATOM | 4142 | CB | LEU | B | 264 | 70.153 | 7.070 | 30.438 | 1.00 | 29.75 | 6 |
| 70 | ATOM | 4143 | CG | LEU | B | 264 | 68.950 | 7.229 | 29.452 | 1.00 | 32.20 | 6 |
| | ATOM | 4144 | CD1 | LEU | B | 264 | 69.399 | 8.095 | 28.298 | 1.00 | 33.01 | 6 |
| | ATOM | 4145 | CD2 | LEU | B | 264 | 68.453 | 5.842 | 29.091 | 1.00 | 31.89 | 6 |
| | ATOM | 4146 | N | VAL | B | 265 | 71.753 | 5.394 | 32.886 | 1.00 | 29.03 | 7 |
| | ATOM | 4147 | CA | VAL | B | 265 | 72.864 | 5.494 | 33.821 | 1.00 | 32.13 | 6 |
| | ATOM | 4148 | C | VAL | B | 265 | 74.099 | 4.822 | 33.213 | 1.00 | 34.01 | 6 |

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|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| | ATOM | 4149 | O | VAL | B | 265 | 74.044 | 3.750 | 32.557 | 1.00 | 34.46 | 8 |
| | ATOM | 4150 | CB | VAL | B | 265 | 72.642 | 4.856 | 35.202 | 1.00 | 32.74 | 6 |
| | ATOM | 4151 | CG1 | VAL | B | 265 | 71.525 | 5.474 | 36.025 | 1.00 | 33.45 | 6 |
| 5 | ATOM | 4152 | CG2 | VAL | B | 265 | 72.331 | 3.361 | 35.046 | 1.00 | 33.30 | 6 |
| | ATOM | 4153 | N | ALA | B | 266 | 75.219 | 5.485 | 33.397 | 1.00 | 33.41 | 7 |
| | ATOM | 4154 | CA | ALA | B | 266 | 76.501 | 4.926 | 33.000 | 1.00 | 32.14 | 6 |
| | ATOM | 4155 | C | ALA | B | 266 | 77.411 | 5.092 | 34.221 | 1.00 | 32.17 | 6 |
| | ATOM | 4156 | O | ALA | B | 266 | 77.390 | 6.213 | 34.746 | 1.00 | 32.13 | 8 |
| 10 | ATOM | 4157 | CB | ALA | B | 266 | 77.139 | 5.570 | 31.794 | 1.00 | 32.99 | 6 |
| | ATOM | 4158 | N | ALA | B | 267 | 78.175 | 4.058 | 34.569 | 1.00 | 31.42 | 7 |
| | ATOM | 4159 | CA | ALA | B | 267 | 79.107 | 4.338 | 35.679 | 1.00 | 32.75 | 6 |
| | ATOM | 4160 | C | ALA | B | 267 | 80.356 | 3.503 | 35.491 | 1.00 | 35.34 | 6 |
| | ATOM | 4161 | O | ALA | B | 267 | 80.213 | 2.423 | 34.884 | 1.00 | 36.90 | 8 |
| 15 | ATOM | 4162 | CB | ALA | B | 267 | 78.446 | 4.006 | 36.993 | 1.00 | 31.22 | 6 |
| | ATOM | 4163 | N | TRP | B | 268 | 81.511 | 3.868 | 36.036 | 1.00 | 36.69 | 7 |
| | ATOM | 4164 | CA | TRP | B | 268 | 82.665 | 2.974 | 35.881 | 1.00 | 38.65 | 6 |
| | ATOM | 4165 | C | TRP | B | 268 | 82.910 | 2.113 | 37.105 | 1.00 | 40.28 | 6 |
| | ATOM | 4166 | O | TRP | B | 268 | 82.777 | 2.579 | 38.235 | 1.00 | 38.57 | 8 |
| 20 | ATOM | 4167 | CB | TRP | B | 268 | 83.927 | 3.805 | 35.609 | 1.00 | 40.65 | 6 |
| | ATOM | 4168 | CG | TRP | B | 268 | 83.860 | 4.563 | 34.319 | 1.00 | 43.80 | 6 |
| | ATOM | 4169 | CD1 | TRP | B | 268 | 83.114 | 5.662 | 34.040 | 1.00 | 44.47 | 6 |
| | ATOM | 4170 | CD2 | TRP | B | 268 | 84.577 | 4.256 | 33.115 | 1.00 | 45.14 | 6 |
| | ATOM | 4171 | NE1 | TRP | B | 268 | 83.311 | 6.063 | 32.729 | 1.00 | 45.41 | 7 |
| 25 | ATOM | 4172 | CE2 | TRP | B | 268 | 84.199 | 5.211 | 32.144 | 1.00 | 45.95 | 6 |
| | ATOM | 4173 | CE3 | TRP | B | 268 | 85.470 | 3.244 | 32.757 | 1.00 | 45.65 | 6 |
| | ATOM | 4174 | CZ2 | TRP | B | 268 | 84.703 | 5.199 | 30.836 | 1.00 | 46.17 | 6 |
| | ATOM | 4175 | CZ3 | TRP | B | 268 | 85.984 | 3.242 | 31.463 | 1.00 | 46.00 | 6 |
| | ATOM | 4176 | CH2 | TRP | B | 268 | 85.596 | 4.206 | 30.522 | 1.00 | 45.63 | 6 |
| 30 | ATOM | 4177 | N | LEU | B | 269 | 83.300 | 0.869 | 36.821 | 1.00 | 39.18 | 7 |
| | ATOM | 4178 | CA | LEU | B | 269 | 83.691 | -0.026 | 37.916 | 1.00 | 43.86 | 6 |
| | ATOM | 4179 | C | LEU | B | 269 | 85.093 | -0.471 | 37.522 | 1.00 | 46.33 | 6 |
| | ATOM | 4180 | O | LEU | B | 269 | 85.247 | -0.946 | 36.400 | 1.00 | 47.07 | 8 |
| | ATOM | 4181 | CB | LEU | B | 269 | 82.635 | -1.086 | 38.058 | 1.00 | 43.77 | 6 |
| 35 | ATOM | 4182 | CG | LEU | B | 269 | 82.651 | -2.072 | 39.212 | 1.00 | 44.62 | 6 |
| | ATOM | 4183 | CD1 | LEU | B | 269 | 82.571 | -1.312 | 40.537 | 1.00 | 44.46 | 6 |
| | ATOM | 4184 | CD2 | LEU | B | 269 | 81.518 | -3.080 | 39.046 | 1.00 | 42.39 | 6 |
| | ATOM | 4185 | N | GLY | B | 270 | 86.102 | -0.049 | 38.293 | 1.00 | 48.41 | 7 |
| | ATOM | 4186 | CA | GLY | B | 270 | 87.475 | -0.340 | 37.862 | 1.00 | 51.49 | 6 |
| 40 | ATOM | 4187 | C | GLY | B | 270 | 87.681 | 0.391 | 36.532 | 1.00 | 54.10 | 6 |
| | ATOM | 4188 | O | GLY | B | 270 | 87.397 | 1.588 | 36.464 | 1.00 | 54.18 | 8 |
| | ATOM | 4189 | N | ASP | B | 271 | 88.108 | -0.331 | 35.503 | 1.00 | 56.24 | 7 |
| | ATOM | 4190 | CA | ASP | B | 271 | 88.288 | 0.320 | 34.199 | 1.00 | 56.89 | 6 |
| | ATOM | 4191 | C | ASP | B | 271 | 87.142 | -0.096 | 33.280 | 1.00 | 54.99 | 6 |
| 45 | ATOM | 4192 | O | ASP | B | 271 | 87.162 | 0.231 | 32.097 | 1.00 | 55.57 | 8 |
| | ATOM | 4193 | CB | ASP | B | 271 | 89.670 | 0.026 | 33.618 | 1.00 | 60.69 | 6 |
| | ATOM | 4194 | CG | ASP | B | 271 | 90.400 | -1.175 | 34.164 | 1.00 | 64.16 | 6 |
| | ATOM | 4195 | OD1 | ASP | B | 271 | 89.789 | -2.194 | 34.571 | 1.00 | 65.71 | 8 |
| | ATOM | 4196 | OD2 | ASP | B | 271 | 91.657 | -1.179 | 34.206 | 1.00 | 66.40 | 8 |
| 50 | ATOM | 4197 | N | ALA | B | 272 | 86.129 | -0.780 | 33.807 | 1.00 | 52.97 | 7 |
| | ATOM | 4198 | CA | ALA | B | 272 | 84.966 | -1.186 | 33.031 | 1.00 | 50.67 | 6 |
| | ATOM | 4199 | C | ALA | B | 272 | 83.843 | -0.149 | 33.103 | 1.00 | 50.64 | 6 |
| | ATOM | 4200 | O | ALA | B | 272 | 83.482 | 0.315 | 34.203 | 1.00 | 49.32 | 8 |
| | ATOM | 4201 | CB | ALA | B | 272 | 84.389 | -2.501 | 33.520 | 1.00 | 50.42 | 6 |
| 55 | ATOM | 4202 | N | ARG | B | 273 | 83.255 | 0.166 | 31.958 | 1.00 | 47.60 | 7 |
| | ATOM | 4203 | CA | ARG | B | 273 | 82.163 | 1.131 | 31.939 | 1.00 | 46.77 | 6 |
| | ATOM | 4204 | C | ARG | B | 273 | 80.841 | 0.398 | 31.804 | 1.00 | 45.84 | 6 |
| | ATOM | 4205 | O | ARG | B | 273 | 80.636 | -0.256 | 30.770 | 1.00 | 46.17 | 8 |
| | ATOM | 4206 | CB | ARG | B | 273 | 82.312 | 2.144 | 30.804 | 1.00 | 48.87 | 6 |
| 60 | ATOM | 4207 | CG | ARG | B | 273 | 81.234 | 3.214 | 30.839 | 1.00 | 49.86 | 6 |
| | ATOM | 4208 | CD | ARG | B | 273 | 81.436 | 4.283 | 29.773 | 1.00 | 52.81 | 6 |
| | ATOM | 4209 | NE | ARG | B | 273 | 80.277 | 5.174 | 29.733 | 1.00 | 54.38 | 7 |
| | ATOM | 4210 | CZ | ARG | B | 273 | 79.665 | 5.669 | 28.671 | 1.00 | 55.34 | 6 |
| | ATOM | 4211 | NH1 | ARG | B | 273 | 80.083 | 5.410 | 27.433 | 1.00 | 56.45 | 7 |
| 65 | ATOM | 4212 | NH2 | ARG | B | 273 | 78.606 | 6.455 | 28.819 | 1.00 | 54.66 | 7 |
| | ATOM | 4213 | N | LEU | B | 274 | 79.992 | 0.448 | 32.821 | 1.00 | 41.38 | 7 |
| | ATOM | 4214 | CA | LEU | B | 274 | 78.715 | -0.229 | 32.792 | 1.00 | 37.98 | 6 |
| | ATOM | 4215 | C | LEU | B | 274 | 77.584 | 0.737 | 32.506 | 1.00 | 37.26 | 6 |
| | ATOM | 4216 | O | LEU | B | 274 | 77.586 | 1.908 | 32.909 | 1.00 | 36.11 | 8 |
| 70 | ATOM | 4217 | CB | LEU | B | 274 | 78.395 | -0.939 | 34.118 | 1.00 | 38.68 | 6 |
| | ATOM | 4218 | CG | LEU | B | 274 | 79.554 | -1.797 | 34.654 | 1.00 | 41.26 | 6 |
| | ATOM | 4219 | CD1 | LEU | B | 274 | 79.161 | -2.469 | 35.960 | 1.00 | 41.73 | 6 |
| | ATOM | 4220 | CD2 | LEU | B | 274 | 79.999 | -2.827 | 33.625 | 1.00 | 42.85 | 6 |
| | ATOM | 4221 | N | ILE | B | 275 | 76.603 | 0.270 | 31.724 | 1.00 | 35.74 | 7 |
| | ATOM | 4222 | CA | ILE | B | 275 | 75.493 | 1.141 | 31.372 | 1.00 | 33.53 | 6 |

-94-

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|----|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|----|
| 5 | ATOM | 4223 | C | ILE | B | 275 | 74.202 | -0.402 | -31.685 | 1.00 | 32.45 | 6 |
| | ATOM | 4224 | O | ILE | B | 275 | 74.121 | -0.836 | 31.733 | 1.00 | 31.50 | 8 |
| | ATOM | 4225 | CB | ILE | B | 275 | 75.466 | 1.658 | 29.914 | 1.00 | 36.92 | 6 |
| | ATOM | 4226 | CG1 | ILE | B | 275 | 75.105 | 0.527 | 28.946 | 1.00 | 37.93 | 6 |
| | ATOM | 4227 | CG2 | ILE | B | 275 | 76.794 | 2.331 | 29.537 | 1.00 | 36.91 | 6 |
| | ATOM | 4228 | CD1 | ILE | B | 275 | 74.962 | 1.004 | 27.506 | 1.00 | 38.53 | 6 |
| | ATOM | 4229 | N | ASP | B | 276 | 73.124 | 1.174 | 31.933 | 1.00 | 28.46 | 7 |
| | ATOM | 4230 | CA | ASP | B | 276 | 71.866 | 0.517 | 32.262 | 1.00 | 30.30 | 6 |
| 10 | ATOM | 4231 | C | ASP | B | 276 | 70.716 | 1.517 | 32.068 | 1.00 | 29.63 | 6 |
| | ATOM | 4232 | O | ASP | B | 276 | 71.081 | 2.666 | 31.835 | 1.00 | 27.88 | 8 |
| | ATOM | 4233 | CB | ASP | B | 276 | 71.937 | -0.066 | 33.671 | 1.00 | 32.97 | 6 |
| | ATOM | 4234 | CG | ASP | B | 276 | 70.851 | -1.058 | 33.987 | 1.00 | 34.63 | 6 |
| | ATOM | 4235 | OD1 | ASP | B | 276 | 69.857 | -1.272 | 33.231 | 1.00 | 37.08 | 8 |
| 15 | ATOM | 4236 | OD2 | ASP | B | 276 | 70.931 | -1.716 | 35.054 | 1.00 | 35.37 | 8 |
| | ATOM | 4237 | N | ASN | B | 277 | 69.478 | 1.072 | 32.012 | 1.00 | 30.76 | 7 |
| | ATOM | 4238 | CA | ASN | B | 277 | 68.339 | 1.963 | 31.738 | 1.00 | 31.92 | 6 |
| | ATOM | 4239 | C | ASN | B | 277 | 67.121 | 1.388 | 32.426 | 1.00 | 29.27 | 6 |
| | ATOM | 4240 | O | ASN | B | 277 | 67.035 | 0.187 | 32.641 | 1.00 | 30.64 | 8 |
| 20 | ATOM | 4241 | CB | ASN | B | 277 | 68.041 | 2.214 | 30.258 | 1.00 | 37.99 | 6 |
| | ATOM | 4242 | CG | ASN | B | 277 | 66.700 | 1.999 | 29.601 | 1.00 | 41.20 | 6 |
| | ATOM | 4243 | OD1 | ASN | B | 277 | 65.702 | 1.397 | 30.046 | 1.00 | 41.98 | 8 |
| | ATOM | 4244 | ND2 | ASN | B | 277 | 66.503 | 2.495 | 28.345 | 1.00 | 41.86 | 7 |
| | ATOM | 4245 | N | LYS | B | 278 | 66.149 | 2.219 | 32.760 | 1.00 | 28.29 | 7 |
| 25 | ATOM | 4246 | CA | LYS | B | 278 | 64.891 | 1.736 | 33.328 | 1.00 | 30.58 | 6 |
| | ATOM | 4247 | C | LYS | B | 278 | 63.822 | 2.756 | 32.929 | 1.00 | 33.32 | 6 |
| | ATOM | 4248 | O | LYS | B | 278 | 64.130 | 3.940 | 32.793 | 1.00 | 32.01 | 8 |
| | ATOM | 4249 | CB | LYS | B | 278 | 64.919 | 1.486 | 34.834 | 1.00 | 31.32 | 6 |
| | ATOM | 4250 | CG | LYS | B | 278 | 63.617 | 0.953 | 35.422 | 1.00 | 35.08 | 6 |
| 30 | ATOM | 4251 | CD | LYS | B | 278 | 63.793 | 0.340 | 36.790 | 1.00 | 38.13 | 6 |
| | ATOM | 4252 | CE | LYS | B | 278 | 63.031 | -0.950 | 37.108 | 1.00 | 39.29 | 6 |
| | ATOM | 4253 | NZ | LYS | B | 278 | 63.193 | -1.103 | 38.612 | 1.00 | 44.44 | 7 |
| | ATOM | 4254 | N | MET | B | 279 | 62.625 | 2.256 | 32.594 | 1.00 | 33.66 | 7 |
| | ATOM | 4255 | CA | MET | B | 279 | 61.488 | 3.102 | 32.303 | 1.00 | 36.39 | 6 |
| 35 | ATOM | 4256 | C | MET | B | 279 | 60.543 | 3.014 | 33.483 | 1.00 | 35.26 | 6 |
| | ATOM | 4257 | O | MET | B | 279 | 60.470 | 1.929 | 34.090 | 1.00 | 38.21 | 8 |
| | ATOM | 4258 | CB | MET | B | 279 | 60.797 | 2.708 | 30.965 | 1.00 | 38.06 | 6 |
| | ATOM | 4259 | CG | MET | B | 279 | 61.358 | 3.604 | 29.846 | 1.00 | 42.01 | 6 |
| | ATOM | 4260 | SD | MET | B | 279 | 61.219 | 2.888 | 28.222 | 1.00 | 48.77 | 16 |
| 40 | ATOM | 4261 | CE | MET | B | 279 | 62.632 | 3.595 | 27.392 | 1.00 | 46.06 | 6 |
| | ATOM | 4262 | N | VAL | B | 280 | 59.853 | 4.082 | 33.859 | 1.00 | 34.69 | 7 |
| | ATOM | 4263 | CA | VAL | B | 280 | 58.937 | 4.046 | 34.991 | 1.00 | 37.86 | 6 |
| | ATOM | 4264 | C | VAL | B | 280 | 57.655 | 4.778 | 34.624 | 1.00 | 39.91 | 6 |
| | ATOM | 4265 | O | VAL | B | 280 | 57.722 | 5.842 | 33.971 | 1.00 | 39.57 | 8 |
| 45 | ATOM | 4266 | CB | VAL | B | 280 | 59.605 | 4.627 | 36.262 | 1.00 | 40.03 | 6 |
| | ATOM | 4267 | CG1 | VAL | B | 280 | 60.582 | 5.734 | 35.894 | 1.00 | 40.43 | 6 |
| | ATOM | 4268 | CG2 | VAL | B | 280 | 58.595 | 5.132 | 37.286 | 1.00 | 41.28 | 6 |
| | ATOM | 4269 | N | GLU | B | 281 | 56.521 | 4.221 | 35.046 | 1.00 | 42.47 | 7 |
| | ATOM | 4270 | CA | GLU | B | 281 | 55.243 | 4.911 | 34.809 | 1.00 | 45.74 | 6 |
| 50 | ATOM | 4271 | C | GLU | B | 281 | 54.973 | 5.919 | 35.910 | 1.00 | 47.07 | 6 |
| | ATOM | 4272 | O | GLU | B | 281 | 55.370 | 5.595 | 37.039 | 1.00 | 46.25 | 8 |
| | ATOM | 4273 | CB | GLU | B | 281 | 54.152 | 3.848 | 34.719 | 1.00 | 47.41 | 6 |
| | ATOM | 4274 | CG | GLU | B | 281 | 54.308 | 2.918 | 33.516 | 1.00 | 48.19 | 6 |
| | ATOM | 4275 | CD | GLU | B | 281 | 53.705 | 3.562 | 32.275 | 1.00 | 50.10 | 6 |
| 55 | ATOM | 4276 | OE1 | GLU | B | 281 | 52.718 | 4.312 | 32.460 | 1.00 | 51.21 | 8 |
| | ATOM | 4277 | OE2 | GLU | B | 281 | 54.203 | 3.330 | 31.153 | 1.00 | 50.72 | 8 |
| | ATOM | 4278 | N | LEU | B | 282 | 54.358 | 7.077 | 35.662 | 1.00 | 49.43 | 7 |
| | ATOM | 4279 | CA | LEU | B | 282 | 54.144 | 8.043 | 36.731 | 1.00 | 52.69 | 6 |
| | ATOM | 4280 | C | LEU | B | 282 | 52.714 | 8.211 | 37.222 | 1.00 | 56.10 | 6 |
| 60 | ATOM | 4281 | O | LEU | B | 282 | 51.741 | 8.259 | 36.479 | 1.00 | 57.86 | 8 |
| | ATOM | 4282 | CB | LEU | B | 282 | 54.654 | 9.413 | 36.232 | 1.00 | 51.33 | 6 |
| | ATOM | 4283 | CG | LEU | B | 282 | 56.153 | 9.442 | 35.898 | 1.00 | 51.16 | 6 |
| | ATOM | 4284 | CD1 | LEU | B | 282 | 56.568 | 10.774 | 35.313 | 1.00 | 49.90 | 6 |
| | ATOM | 4285 | CD2 | LEU | B | 282 | 56.959 | 9.109 | 37.146 | 1.00 | 50.87 | 6 |
| 65 | ATOM | 4286 | N | ALA | B | 283 | 52.591 | 8.404 | 38.527 | 1.00 | 58.60 | 7 |
| | ATOM | 4287 | CA | ALA | B | 283 | 51.340 | 8.572 | 39.260 | 1.00 | 61.51 | 6 |
| | ATOM | 4288 | C | ALA | B | 283 | 50.222 | 7.659 | 38.748 | 1.00 | 62.69 | 6 |
| | ATOM | 4289 | O | ALA | B | 283 | 49.365 | 7.240 | 39.565 | 1.00 | 64.21 | 8 |
| 70 | ATOM | 4290 | CB | ALA | B | 283 | 50.878 | 10.031 | 39.215 | 1.00 | 61.28 | |

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|------|---|---|---|------|---|
| Atom | X | Y | Z | Occ. | B |
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|----|------|------|---|-----|---|----|--------|---------|---------|------|-------|
| | ATOM | 4303 | O | WAT | W | 1 | 33.957 | 17.885 | -21.689 | 1.00 | 20.48 |
| 5 | ATOM | 4304 | O | WAT | W | 2 | 37.847 | 13.185 | 4.982 | 1.00 | 21.45 |
| | ATOM | 4305 | O | WAT | W | 3 | 63.980 | -1.350 | 11.191 | 1.00 | 28.46 |
| | ATOM | 4306 | O | WAT | W | 4 | 56.095 | -1.331 | -2.328 | 1.00 | 33.26 |
| | ATOM | 4307 | O | WAT | W | 5 | 33.170 | 18.137 | -24.293 | 1.00 | 23.96 |
| | ATOM | 4308 | O | WAT | W | 6 | 37.215 | 10.622 | -2.497 | 1.00 | 25.23 |
| 10 | ATOM | 4309 | O | WAT | W | 7 | 34.408 | 20.030 | -20.099 | 1.00 | 22.90 |
| | ATOM | 4310 | O | WAT | W | 8 | 44.843 | 0.417 | 12.211 | 1.00 | 25.44 |
| | ATOM | 4311 | O | WAT | W | 9 | 32.057 | 20.794 | -18.723 | 1.00 | 21.33 |
| | ATOM | 4312 | O | WAT | W | 10 | 39.891 | 15.086 | 5.128 | 1.00 | 21.17 |
| | ATOM | 4313 | O | WAT | W | 11 | 60.554 | 9.975 | 11.882 | 1.00 | 23.86 |
| 15 | ATOM | 4314 | O | WAT | W | 12 | 47.956 | 16.767 | 16.754 | 1.00 | 25.70 |
| | ATOM | 4315 | O | WAT | W | 13 | 26.013 | 19.028 | 0.123 | 1.00 | 29.25 |
| | ATOM | 4316 | O | WAT | W | 14 | 41.289 | 15.802 | -0.016 | 1.00 | 29.45 |
| | ATOM | 4317 | O | WAT | W | 15 | 26.238 | 26.828 | -12.429 | 1.00 | 26.43 |
| | ATOM | 4318 | O | WAT | W | 16 | 42.677 | -8.069 | 14.438 | 1.00 | 49.57 |
| 20 | ATOM | 4319 | O | WAT | W | 17 | 44.205 | -22.405 | 7.937 | 1.00 | 26.54 |
| | ATOM | 4320 | O | WAT | W | 18 | 41.204 | 15.438 | 2.596 | 1.00 | 28.73 |
| | ATOM | 4321 | O | WAT | W | 19 | 50.665 | 6.851 | -9.161 | 1.00 | 28.82 |
| | ATOM | 4322 | O | WAT | W | 20 | 45.856 | 11.020 | 16.763 | 1.00 | 28.19 |
| | ATOM | 4323 | O | WAT | W | 21 | 56.240 | 9.146 | 22.228 | 1.00 | 29.25 |
| 25 | ATOM | 4324 | O | WAT | W | 22 | 34.167 | 22.025 | -17.131 | 1.00 | 24.52 |
| | ATOM | 4325 | O | WAT | W | 23 | 46.937 | -3.706 | 12.756 | 1.00 | 34.74 |
| | ATOM | 4326 | O | WAT | W | 24 | 42.413 | 2.422 | 14.402 | 1.00 | 33.61 |
| | ATOM | 4327 | O | WAT | W | 25 | 41.229 | -21.204 | 14.206 | 1.00 | 24.13 |
| | ATOM | 4328 | O | WAT | W | 26 | 41.221 | 12.093 | -6.937 | 1.00 | 25.26 |
| 30 | ATOM | 4329 | O | WAT | W | 27 | 24.372 | 15.958 | -5.041 | 1.00 | 27.65 |
| | ATOM | 4330 | O | WAT | W | 28 | 35.615 | -12.052 | 11.939 | 1.00 | 30.34 |
| | ATOM | 4331 | O | WAT | W | 29 | 37.895 | 12.192 | -4.849 | 1.00 | 26.69 |
| | ATOM | 4332 | O | WAT | W | 30 | 52.106 | 20.252 | -2.182 | 1.00 | 28.30 |
| | ATOM | 4333 | O | WAT | W | 31 | 68.369 | 9.094 | 44.468 | 1.00 | 25.44 |
| 35 | ATOM | 4334 | O | WAT | W | 32 | 56.344 | 0.572 | -4.129 | 1.00 | 43.47 |
| | ATOM | 4335 | O | WAT | W | 33 | 23.101 | 20.797 | -4.005 | 1.00 | 36.59 |
| | ATOM | 4336 | O | WAT | W | 34 | 49.261 | -5.331 | 2.868 | 1.00 | 26.99 |
| | ATOM | 4337 | O | WAT | W | 35 | 47.984 | -9.414 | 25.007 | 1.00 | 26.83 |
| | ATOM | 4338 | O | WAT | W | 36 | 42.604 | -1.487 | 5.352 | 1.00 | 30.62 |
| 40 | ATOM | 4339 | O | WAT | W | 37 | 62.274 | -5.597 | 10.141 | 1.00 | 27.42 |
| | ATOM | 4340 | O | WAT | W | 38 | 26.216 | 16.962 | -12.131 | 1.00 | 28.51 |
| | ATOM | 4341 | O | WAT | W | 39 | 30.958 | 20.957 | -10.945 | 1.00 | 28.67 |
| | ATOM | 4342 | O | WAT | W | 40 | 34.816 | 15.313 | 17.023 | 1.00 | 30.79 |
| | ATOM | 4343 | O | WAT | W | 41 | 49.918 | 15.022 | 17.578 | 1.00 | 28.50 |
| 45 | ATOM | 4344 | O | WAT | W | 42 | 51.910 | 5.889 | 8.625 | 1.00 | 38.44 |
| | ATOM | 4345 | O | WAT | W | 43 | 62.846 | -1.187 | 14.226 | 1.00 | 46.50 |
| | ATOM | 4346 | O | WAT | W | 44 | 25.403 | 26.593 | -16.292 | 1.00 | 39.06 |
| | ATOM | 4347 | O | WAT | W | 45 | 30.520 | 20.301 | 5.385 | 1.00 | 32.49 |
| | ATOM | 4348 | O | WAT | W | 46 | 45.010 | -17.167 | 2.635 | 1.00 | 34.22 |
| 50 | ATOM | 4349 | O | WAT | W | 47 | 47.032 | -2.770 | 5.031 | 1.00 | 22.23 |
| | ATOM | 4350 | O | WAT | W | 48 | 48.414 | 1.477 | -5.713 | 1.00 | 29.51 |
| | ATOM | 4351 | O | WAT | W | 49 | 31.672 | 7.463 | -13.621 | 1.00 | 36.04 |
| | ATOM | 4352 | O | WAT | W | 50 | 62.969 | 0.366 | 20.839 | 1.00 | 25.12 |
| | ATOM | 4353 | O | WAT | W | 51 | 52.181 | 16.341 | 18.209 | 1.00 | 33.67 |
| 55 | ATOM | 4354 | O | WAT | W | 52 | 34.216 | 17.207 | 10.342 | 1.00 | 25.68 |
| | ATOM | 4355 | O | WAT | W | 53 | 52.739 | 13.892 | -0.142 | 1.00 | 24.81 |
| | ATOM | 4356 | O | WAT | W | 54 | 48.513 | -7.403 | 4.595 | 1.00 | 33.10 |
| | ATOM | 4357 | O | WAT | W | 55 | 50.165 | 3.786 | 7.424 | 1.00 | 31.96 |
| | ATOM | 4358 | O | WAT | W | 56 | 61.601 | -10.884 | -3.900 | 1.00 | 38.55 |
| 60 | ATOM | 4359 | O | WAT | W | 57 | 40.862 | -13.477 | 5.834 | 1.00 | 26.78 |
| | ATOM | 4360 | O | WAT | W | 58 | 73.540 | -3.703 | 38.069 | 1.00 | 28.56 |
| | ATOM | 4361 | O | WAT | W | 59 | 53.267 | 18.858 | -0.006 | 1.00 | 28.15 |
| | ATOM | 4362 | O | WAT | W | 60 | 47.896 | -10.104 | 11.452 | 1.00 | 29.42 |
| | ATOM | 4363 | O | WAT | W | 61 | 32.210 | 13.233 | -12.282 | 1.00 | 31.94 |
| 65 | ATOM | 4364 | O | WAT | W | 62 | 48.007 | 11.908 | 18.269 | 1.00 | 37.69 |
| | ATOM | 4365 | O | WAT | W | 63 | 29.173 | 9.259 | -17.716 | 1.00 | 30.38 |
| | ATOM | 4366 | O | WAT | W | 64 | 35.297 | 19.389 | 9.031 | 1.00 | 29.80 |
| | ATOM | 4367 | O | WAT | W | 65 | 40.504 | 2.299 | -10.545 | 1.00 | 32.49 |
| | ATOM | 4368 | O | WAT | W | 66 | 41.958 | -10.772 | 13.351 | 1.00 | 42.64 |
| 70 | ATOM | 4369 | O | WAT | W | 67 | 36.143 | 16.525 | -1.066 | 1.00 | 34.59 |
| | ATOM | 4370 | O | WAT | W | 68 | 62.385 | -11.067 | -1.312 | 1.00 | 33.16 |
| | ATOM | 4371 | O | WAT | W | 69 | 65.110 | 11.392 | 10.350 | 1.00 | 28.97 |
| | ATOM | 4372 | O | WAT | W | 70 | 63.427 | -3.415 | 19.364 | 1.00 | 27.45 |
| | ATOM | 4373 | O | WAT | W | 71 | 68.617 | 14.525 | 33.511 | 1.00 | 37.55 |
| | ATOM | 4374 | O | WAT | W | 72 | 61.639 | -4.893 | 17.918 | 1.00 | 24.98 |

-96-

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|----|------|------|---|-----|---|-----|--------|---------|---------|------|-------|
| | ATOM | 4375 | O | WAT | W | 73 | 66.736 | 4.204 | 19.794 | 1.00 | 30.21 |
| | ATOM | 4376 | O | WAT | W | 74 | 55.982 | 12.796 | 22.001 | 1.00 | 36.21 |
| | ATOM | 4377 | O | WAT | W | 75 | 64.346 | 6.123 | -5.386 | 1.00 | 40.37 |
| 5 | ATOM | 4378 | O | WAT | W | 76 | 65.025 | -2.313 | 32.956 | 1.00 | 37.41 |
| | ATOM | 4379 | O | WAT | W | 77 | 44.448 | -0.359 | -6.294 | 1.00 | 29.00 |
| | ATOM | 4380 | O | WAT | W | 78 | 48.675 | -0.966 | -4.566 | 1.00 | 35.26 |
| | ATOM | 4381 | O | WAT | W | 79 | 31.748 | 14.620 | -27.469 | 1.00 | 30.01 |
| | ATOM | 4382 | O | WAT | W | 80 | 22.272 | 14.300 | -4.370 | 1.00 | 33.41 |
| 10 | ATOM | 4383 | O | WAT | W | 81 | 61.185 | 6.162 | 25.319 | 1.00 | 33.42 |
| | ATOM | 4384 | O | WAT | W | 82 | 25.793 | 11.693 | -9.261 | 1.00 | 32.09 |
| | ATOM | 4385 | O | WAT | W | 83 | 44.087 | 16.403 | -7.636 | 1.00 | 30.17 |
| | ATOM | 4386 | O | WAT | W | 84 | 42.576 | -4.126 | 6.016 | 1.00 | 55.25 |
| | ATOM | 4387 | O | WAT | W | 85 | 68.891 | 7.733 | 20.798 | 1.00 | 37.85 |
| 15 | ATOM | 4388 | O | WAT | W | 86 | 70.712 | -5.611 | 41.295 | 1.00 | 34.04 |
| | ATOM | 4389 | O | WAT | W | 87 | 43.384 | -22.647 | 14.391 | 1.00 | 41.78 |
| | ATOM | 4390 | O | WAT | W | 88 | 70.983 | -8.966 | 9.646 | 1.00 | 33.63 |
| | ATOM | 4391 | O | WAT | W | 89 | 75.957 | -17.895 | 11.852 | 1.00 | 47.71 |
| | ATOM | 4392 | O | WAT | W | 90 | 63.730 | -0.759 | 18.432 | 1.00 | 34.78 |
| 20 | ATOM | 4393 | O | WAT | W | 91 | 31.689 | 15.534 | -14.467 | 1.00 | 32.23 |
| | ATOM | 4394 | O | WAT | W | 92 | 44.527 | -11.830 | 12.755 | 1.00 | 34.17 |
| | ATOM | 4395 | O | WAT | W | 93 | 20.677 | 30.620 | -24.626 | 1.00 | 31.71 |
| | ATOM | 4396 | O | WAT | W | 94 | 44.639 | 17.338 | -10.200 | 1.00 | 34.48 |
| | ATOM | 4397 | O | WAT | W | 95 | 75.731 | 12.312 | 36.456 | 1.00 | 43.57 |
| 25 | ATOM | 4398 | O | WAT | W | 96 | 44.412 | 10.904 | 19.269 | 1.00 | 42.19 |
| | ATOM | 4399 | O | WAT | W | 97 | 22.294 | 30.665 | -27.831 | 1.00 | 34.67 |
| | ATOM | 4400 | O | WAT | W | 98 | 61.020 | 1.839 | -4.047 | 1.00 | 32.70 |
| | ATOM | 4401 | O | WAT | W | 99 | 63.564 | -3.241 | 9.033 | 1.00 | 26.37 |
| | ATOM | 4402 | O | WAT | W | 100 | 58.754 | 3.167 | -4.838 | 1.00 | 32.36 |
| 30 | ATOM | 4403 | O | WAT | W | 101 | 65.772 | -9.474 | 4.700 | 1.00 | 28.90 |
| | ATOM | 4404 | O | WAT | W | 102 | 68.154 | 15.020 | 30.966 | 1.00 | 48.55 |
| | ATOM | 4405 | O | WAT | W | 103 | 69.423 | 3.142 | 26.541 | 1.00 | 37.38 |
| | ATOM | 4406 | O | WAT | W | 104 | 46.011 | 16.393 | -32.096 | 1.00 | 35.12 |
| | ATOM | 4407 | O | WAT | W | 105 | 29.379 | 18.412 | -31.086 | 1.00 | 39.01 |
| 35 | ATOM | 4408 | O | WAT | W | 106 | 45.917 | -11.276 | 10.149 | 1.00 | 27.62 |
| | ATOM | 4409 | O | WAT | W | 107 | 24.739 | 28.644 | -17.280 | 1.00 | 32.77 |
| | ATOM | 4410 | O | WAT | W | 108 | 79.205 | 12.257 | 45.859 | 1.00 | 41.16 |
| | ATOM | 4411 | O | WAT | W | 109 | 73.058 | -3.265 | 35.431 | 1.00 | 33.63 |
| | ATOM | 4412 | O | WAT | W | 110 | 46.854 | -9.240 | 3.826 | 1.00 | 36.79 |
| 40 | ATOM | 4413 | O | WAT | W | 111 | 25.850 | 9.001 | -9.625 | 1.00 | 34.69 |
| | ATOM | 4414 | O | WAT | W | 112 | 62.047 | 8.655 | 0.423 | 1.00 | 33.56 |
| | ATOM | 4415 | O | WAT | W | 113 | 37.663 | 10.928 | -18.842 | 1.00 | 34.05 |
| | ATOM | 4416 | O | WAT | W | 114 | 34.619 | 21.383 | -14.295 | 1.00 | 30.74 |
| | ATOM | 4417 | O | WAT | W | 115 | 58.523 | 21.835 | -8.875 | 1.00 | 37.34 |
| 45 | ATOM | 4418 | O | WAT | W | 116 | 28.178 | 28.182 | -10.656 | 1.00 | 43.64 |
| | ATOM | 4419 | O | WAT | W | 117 | 66.395 | -3.417 | 24.653 | 1.00 | 32.24 |
| | ATOM | 4420 | O | WAT | W | 118 | 51.651 | 21.138 | 16.503 | 1.00 | 35.04 |
| | ATOM | 4421 | O | WAT | W | 119 | 46.184 | -9.790 | 13.725 | 1.00 | 38.61 |
| | ATOM | 4422 | O | WAT | W | 120 | 77.317 | -2.960 | 44.894 | 1.00 | 29.27 |
| 50 | ATOM | 4423 | O | WAT | W | 121 | 53.189 | 17.937 | 10.605 | 1.00 | 29.73 |
| | ATOM | 4424 | O | WAT | W | 122 | 36.010 | 12.829 | -10.679 | 1.00 | 33.47 |
| | ATOM | 4425 | O | WAT | W | 123 | 34.086 | 3.401 | -11.327 | 1.00 | 50.83 |
| | ATOM | 4426 | O | WAT | W | 124 | 67.551 | -6.941 | -3.458 | 1.00 | 40.00 |
| | ATOM | 4427 | O | WAT | W | 125 | 22.839 | 14.210 | -21.134 | 1.00 | 33.56 |
| 55 | ATOM | 4428 | O | WAT | W | 126 | 46.144 | 1.450 | -7.279 | 1.00 | 34.78 |
| | ATOM | 4429 | O | WAT | W | 127 | 44.101 | 21.525 | 16.698 | 1.00 | 39.31 |
| | ATOM | 4430 | O | WAT | W | 128 | 53.306 | 5.434 | -16.838 | 1.00 | 54.57 |
| | ATOM | 4431 | O | WAT | W | 129 | 50.250 | 1.205 | 22.740 | 1.00 | 28.98 |
| | ATOM | 4432 | O | WAT | W | 130 | 26.485 | 19.155 | -29.949 | 1.00 | 29.98 |
| 60 | ATOM | 4433 | O | WAT | W | 131 | 24.707 | 18.542 | -27.822 | 1.00 | 37.35 |
| | ATOM | 4434 | O | WAT | W | 132 | 67.710 | 5.567 | 21.896 | 1.00 | 29.04 |
| | ATOM | 4435 | O | WAT | W | 133 | 45.674 | -4.052 | 19.840 | 1.00 | 36.16 |
| | ATOM | 4436 | O | WAT | W | 134 | 24.220 | 25.124 | -21.068 | 1.00 | 34.59 |
| | ATOM | 4437 | O | WAT | W | 135 | 61.598 | 17.680 | 13.540 | 1.00 | 42.71 |
| 65 | ATOM | 4438 | O | WAT | W | 136 | 49.468 | -7.110 | 25.310 | 1.00 | 38.94 |
| | ATOM | 4439 | O | WAT | W | 137 | 66.911 | 11.234 | 12.429 | 1.00 | 37.05 |
| | ATOM | 4440 | O | WAT | W | 138 | 57.148 | 2.737 | 30.896 | 1.00 | 48.38 |
| | ATOM | 4441 | O | WAT | W | 139 | 34.489 | 9.771 | -18.467 | 1.00 | 30.91 |
| | ATOM | 4442 | O | WAT | W | 140 | 32.760 | 21.132 | 4.304 | 1.00 | 29.66 |
| 70 | ATOM | 4443 | O | WAT | W | 141 | 49.857 | -2.000 | -1.297 | 1.00 | 39.89 |
| | ATOM | 4444 | O | WAT | W | 142 | 54.890 | -1.411 | 27.207 | 1.00 | 47.87 |
| | ATOM | 4445 | O | WAT | W | 143 | 64.172 | 15.675 | 32.993 | 1.00 | 36.07 |
| | ATOM | 4446 | O | WAT | W | 144 | 55.868 | -7.470 | -4.555 | 1.00 | 42.27 |
| | ATOM | 4447 | O | WAT | W | 145 | 44.776 | 21.855 | -19.009 | 1.00 | 46.18 |
| | ATOM | 4448 | O | WAT | W | 146 | 81.842 | 9.124 | 42.112 | 1.00 | 41.17 |

-97-

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|----|------|------|---|-----------|--------|---------|---------|------|-------|
| | ATOM | 4449 | O | WAT W 147 | 65.891 | 12.184 | 46.900 | 1.00 | 41.27 |
| | ATOM | 4450 | O | WAT W 148 | 61.870 | -0.694 | 32.618 | 1.00 | 36.54 |
| | ATOM | 4451 | O | WAT W 149 | 53.665 | -22.423 | 14.114 | 1.00 | 45.13 |
| 5 | ATOM | 4452 | O | WAT W 150 | 70.406 | -11.509 | 9.153 | 1.00 | 39.16 |
| | ATOM | 4453 | O | WAT W 151 | 57.272 | 24.770 | -5.465 | 1.00 | 53.97 |
| | ATOM | 4454 | O | WAT W 152 | 76.932 | 13.052 | 43.714 | 1.00 | 34.28 |
| | ATOM | 4455 | O | WAT W 153 | 46.722 | -10.271 | 21.629 | 1.00 | 39.60 |
| | ATOM | 4456 | O | WAT W 154 | 71.871 | -14.779 | 14.884 | 1.00 | 41.12 |
| 10 | ATOM | 4457 | O | WAT W 155 | 75.221 | -2.490 | 33.675 | 1.00 | 36.01 |
| | ATOM | 4458 | O | WAT W 156 | 79.538 | 8.216 | 41.312 | 1.00 | 39.15 |
| | ATOM | 4459 | O | WAT W 157 | 37.416 | -3.706 | 5.762 | 1.00 | 38.40 |
| | ATOM | 4460 | O | WAT W 158 | 35.517 | 15.310 | 19.620 | 1.00 | 36.39 |
| | ATOM | 4461 | O | WAT W 159 | 51.237 | 5.731 | 5.785 | 1.00 | 34.79 |
| 15 | ATOM | 4462 | O | WAT W 160 | 51.381 | -1.632 | 26.211 | 1.00 | 44.45 |
| | ATOM | 4463 | O | WAT W 161 | 43.466 | 16.232 | -32.007 | 1.00 | 52.60 |
| | ATOM | 4464 | O | WAT W 162 | 75.662 | 12.257 | 40.222 | 1.00 | 38.37 |
| | ATOM | 4465 | O | WAT W 163 | 32.057 | -13.026 | 10.708 | 1.00 | 39.45 |
| | ATOM | 4466 | O | WAT W 164 | 44.346 | 0.072 | 6.468 | 1.00 | 36.40 |
| 20 | ATOM | 4467 | O | WAT W 165 | 52.324 | -2.560 | -1.704 | 1.00 | 46.60 |
| | ATOM | 4468 | O | WAT W 166 | 57.861 | 8.649 | -15.458 | 1.00 | 41.61 |
| | ATOM | 4469 | O | WAT W 167 | 67.132 | -5.044 | 15.257 | 1.00 | 40.23 |
| | ATOM | 4470 | O | WAT W 168 | 59.264 | -1.197 | 31.588 | 1.00 | 51.30 |
| | ATOM | 4471 | O | WAT W 169 | 51.835 | 3.346 | 23.021 | 1.00 | 39.67 |
| 25 | ATOM | 4472 | O | WAT W 170 | 57.419 | -5.177 | -4.443 | 1.00 | 35.72 |
| | ATOM | 4473 | O | WAT W 171 | 48.627 | 11.775 | 20.770 | 1.00 | 47.02 |
| | ATOM | 4474 | O | WAT W 172 | 64.778 | -5.263 | 25.321 | 1.00 | 34.04 |
| | ATOM | 4475 | O | WAT W 173 | 21.644 | 11.926 | -2.423 | 1.00 | 35.54 |
| | ATOM | 4476 | O | WAT W 174 | 40.345 | 0.581 | 13.671 | 1.00 | 59.11 |
| 30 | ATOM | 4477 | O | WAT W 175 | 65.019 | -5.440 | 32.798 | 1.00 | 40.87 |
| | ATOM | 4478 | O | WAT W 176 | 44.228 | -7.202 | 4.474 | 1.00 | 39.61 |
| | ATOM | 4479 | O | WAT W 177 | 83.719 | 10.000 | 40.277 | 1.00 | 42.80 |
| | ATOM | 4480 | O | WAT W 178 | 68.408 | -7.591 | -0.478 | 1.00 | 38.18 |
| | ATOM | 4481 | O | WAT W 179 | 63.973 | -9.992 | -4.755 | 1.00 | 51.42 |
| 35 | ATOM | 4482 | O | WAT W 180 | 39.726 | 7.902 | -27.189 | 1.00 | 49.92 |
| | ATOM | 4483 | O | WAT W 181 | 55.044 | 0.850 | -6.811 | 1.00 | 51.09 |
| | ATOM | 4484 | O | WAT W 182 | 25.424 | 1.610 | -6.315 | 1.00 | 30.30 |
| | ATOM | 4485 | O | WAT W 183 | 25.655 | 20.392 | -3.870 | 1.00 | 43.57 |
| | ATOM | 4486 | O | WAT W 184 | 43.760 | -10.333 | 15.054 | 1.00 | 39.92 |
| 40 | ATOM | 4487 | O | WAT W 185 | 46.383 | 19.180 | -9.597 | 1.00 | 33.30 |
| | ATOM | 4488 | O | WAT W 186 | 57.924 | 9.404 | -18.120 | 1.00 | 44.22 |
| | ATOM | 4489 | O | WAT W 187 | 58.234 | -16.451 | 0.308 | 1.00 | 36.17 |
| | ATOM | 4490 | O | WAT W 188 | 38.059 | -19.859 | 11.817 | 1.00 | 32.02 |
| | ATOM | 4491 | O | WAT W 189 | 42.349 | 23.603 | 0.069 | 1.00 | 55.22 |
| 45 | ATOM | 4492 | O | WAT W 190 | 62.117 | 0.301 | 41.059 | 1.00 | 47.46 |
| | ATOM | 4493 | O | WAT W 191 | 39.146 | 34.096 | 6.333 | 1.00 | 35.61 |
| | ATOM | 4494 | O | WAT W 192 | 52.021 | -17.641 | 1.723 | 1.00 | 36.52 |
| | ATOM | 4495 | O | WAT W 193 | 30.405 | 15.315 | -12.140 | 1.00 | 40.90 |
| | ATOM | 4496 | O | WAT W 194 | 56.589 | 6.376 | -25.137 | 1.00 | 50.29 |
| 50 | ATOM | 4497 | O | WAT W 195 | 32.292 | 21.747 | -31.418 | 1.00 | 30.10 |
| | ATOM | 4498 | O | WAT W 196 | 25.932 | 26.262 | -31.876 | 1.00 | 33.19 |
| | ATOM | 4499 | O | WAT W 197 | 44.253 | 27.169 | 0.607 | 1.00 | 41.25 |
| | ATOM | 4500 | O | WAT W 198 | 31.985 | 18.702 | 10.898 | 1.00 | 43.36 |
| | ATOM | 4501 | O | WAT W 199 | 66.104 | 14.551 | 9.666 | 1.00 | 42.15 |
| 55 | ATOM | 4502 | O | WAT W 200 | 65.400 | 14.447 | 48.384 | 1.00 | 54.11 |
| | ATOM | 4503 | O | WAT W 201 | 23.164 | 26.745 | -32.350 | 1.00 | 43.78 |
| | ATOM | 4504 | O | WAT W 202 | 36.449 | -19.529 | 9.775 | 1.00 | 56.52 |
| | ATOM | 4505 | O | WAT W 203 | 37.955 | 9.830 | -30.717 | 1.00 | 42.18 |
| | ATOM | 4506 | O | WAT W 204 | 80.612 | -6.612 | 30.354 | 1.00 | 58.09 |
| 60 | ATOM | 4507 | O | WAT W 205 | 42.193 | -5.177 | 3.641 | 1.00 | 53.40 |
| | ATOM | 4508 | O | WAT W 206 | 34.846 | 19.253 | -0.441 | 1.00 | 43.51 |
| | ATOM | 4509 | O | WAT W 207 | 55.615 | -2.982 | -4.231 | 1.00 | 46.41 |
| | ATOM | 4510 | O | WAT W 208 | 51.625 | 4.220 | -8.519 | 1.00 | 45.10 |
| | ATOM | 4511 | O | WAT W 209 | 25.739 | 8.524 | -24.942 | 1.00 | 36.13 |
| 65 | ATOM | 4512 | O | WAT W 210 | 68.747 | 17.314 | 21.066 | 1.00 | 43.56 |
| | ATOM | 4513 | O | WAT W 211 | 84.666 | 3.989 | 47.339 | 1.00 | 56.35 |
| | ATOM | 4514 | O | WAT W 212 | 39.125 | 28.472 | 0.851 | 1.00 | 43.49 |
| | ATOM | 4515 | O | WAT W 213 | 40.758 | -6.436 | 1.126 | 1.00 | 43.08 |
| | ATOM | 4516 | O | WAT W 214 | 65.742 | -7.673 | 25.260 | 1.00 | 39.84 |
| 70 | ATOM | 4517 | O | WAT W 215 | 68.113 | -7.014 | 26.268 | 1.00 | 44.06 |
| | ATOM | 4518 | O | WAT W 216 | 50.292 | 24.666 | -37.803 | 1.00 | 47.27 |
| | ATOM | 4519 | O | WAT W 217 | 76.215 | -4.709 | 32.421 | 1.00 | 35.98 |
| | ATOM | 4520 | O | WAT W 218 | 28.732 | 31.945 | -22.056 | 1.00 | 33.29 |
| | ATOM | 4521 | O | WAT W 219 | 74.218 | 14.100 | 34.912 | 1.00 | 76.11 |
| | ATOM | 4522 | O | WAT W 220 | 57.961 | 0.451 | 28.074 | 1.00 | 47.45 |

-98-

| | | | | | | | | | | | |
|----|------|------|---|-----|---|-----|--------|---------|---------|------|-------|
| | ATOM | 4523 | O | WAT | W | 221 | 32.590 | 10.932 | -11.111 | 1.00 | 49.96 |
| | ATOM | 4524 | O | WAT | W | 222 | 51.203 | -19.722 | 11.498 | 1.00 | 41.52 |
| | ATOM | 4525 | O | WAT | W | 223 | 55.448 | -14.143 | -4.633 | 1.00 | 36.90 |
| 5 | ATOM | 4526 | O | WAT | W | 224 | 21.981 | 23.670 | -26.954 | 1.00 | 35.03 |
| | ATOM | 4527 | O | WAT | W | 225 | 38.572 | -13.668 | 7.579 | 1.00 | 39.66 |
| | ATOM | 4528 | O | WAT | W | 226 | 56.707 | -16.581 | 26.316 | 1.00 | 35.78 |
| | ATOM | 4529 | O | WAT | W | 227 | 70.225 | 2.519 | 46.317 | 1.00 | 45.99 |
| | ATOM | 4530 | O | WAT | W | 228 | 36.498 | 21.585 | 14.126 | 1.00 | 33.98 |
| 10 | ATOM | 4531 | O | WAT | W | 229 | 61.790 | -13.520 | -4.514 | 1.00 | 50.15 |
| | ATOM | 4532 | O | WAT | W | 230 | 64.989 | -1.584 | 30.303 | 1.00 | 36.47 |
| | ATOM | 4533 | O | WAT | W | 231 | 38.229 | 27.188 | 10.218 | 1.00 | 45.56 |
| | ATOM | 4534 | O | WAT | W | 232 | 67.835 | -7.729 | 5.083 | 1.00 | 34.03 |
| | ATOM | 4535 | O | WAT | W | 233 | 45.674 | 22.663 | 18.801 | 1.00 | 65.84 |
| 15 | ATOM | 4536 | O | WAT | W | 234 | 43.579 | -5.428 | 17.882 | 1.00 | 43.49 |
| | ATOM | 4537 | O | WAT | W | 235 | 64.221 | 5.067 | 46.860 | 1.00 | 41.97 |
| | ATOM | 4538 | O | WAT | W | 236 | 72.469 | 18.804 | 43.000 | 1.00 | 36.08 |
| | ATOM | 4539 | O | WAT | W | 237 | 43.180 | 3.609 | 16.574 | 1.00 | 59.75 |
| | ATOM | 4540 | O | WAT | W | 238 | 34.121 | 16.290 | -13.499 | 1.00 | 46.11 |
| 20 | ATOM | 4541 | O | WAT | W | 239 | 62.037 | 17.693 | 20.122 | 1.00 | 50.69 |
| | ATOM | 4542 | O | WAT | W | 240 | 37.376 | 10.472 | -16.234 | 1.00 | 45.81 |
| | ATOM | 4543 | O | WAT | W | 241 | 26.431 | 22.009 | -0.233 | 1.00 | 46.92 |
| | ATOM | 4544 | O | WAT | W | 242 | 25.310 | 12.750 | -11.978 | 1.00 | 50.59 |
| | ATOM | 4545 | O | WAT | W | 243 | 19.671 | 9.916 | -3.708 | 1.00 | 49.70 |
| 25 | ATOM | 4546 | O | WAT | W | 244 | 38.186 | 21.703 | 16.967 | 1.00 | 35.43 |
| | ATOM | 4547 | O | WAT | W | 245 | 40.977 | -0.520 | -8.992 | 1.00 | 51.53 |
| | ATOM | 4548 | O | WAT | W | 246 | 17.264 | 17.138 | 1.436 | 1.00 | 65.65 |
| | ATOM | 4549 | O | WAT | W | 247 | 59.212 | -16.788 | -2.401 | 1.00 | 43.21 |
| | ATOM | 4550 | O | WAT | W | 248 | 77.330 | -11.434 | 7.852 | 1.00 | 51.89 |
| 30 | ATOM | 4551 | O | WAT | W | 249 | 22.908 | 25.131 | -34.628 | 1.00 | 44.65 |
| | ATOM | 4552 | O | WAT | W | 250 | 37.272 | 2.059 | 20.950 | 1.00 | 42.62 |
| | ATOM | 4553 | O | WAT | W | 251 | 78.365 | -12.406 | 10.087 | 1.00 | 55.28 |
| | ATOM | 4554 | O | WAT | W | 252 | 31.173 | 17.182 | -10.252 | 1.00 | 47.60 |
| | ATOM | 4555 | O | WAT | W | 253 | 48.516 | -12.376 | -1.883 | 1.00 | 33.36 |
| 35 | ATOM | 4556 | O | WAT | W | 254 | 43.940 | 18.919 | -6.022 | 1.00 | 54.48 |
| | ATOM | 4557 | O | WAT | W | 255 | 30.610 | 3.062 | 18.104 | 1.00 | 46.62 |
| | ATOM | 4558 | O | WAT | W | 256 | 72.364 | 2.032 | 11.881 | 1.00 | 60.78 |
| | ATOM | 4559 | O | WAT | W | 257 | 36.491 | -6.172 | 6.630 | 1.00 | 48.36 |
| | ATOM | 4560 | O | WAT | W | 258 | 65.789 | -10.191 | 31.731 | 1.00 | 42.15 |
| 40 | ATOM | 4561 | O | WAT | W | 259 | 59.438 | 15.957 | 21.720 | 1.00 | 40.75 |
| | ATOM | 4562 | O | WAT | W | 260 | 31.766 | 20.345 | 7.940 | 1.00 | 41.46 |
| | ATOM | 4563 | O | WAT | W | 261 | 38.175 | 22.668 | 9.740 | 1.00 | 36.51 |
| | ATOM | 4564 | O | WAT | W | 262 | 69.731 | 20.766 | 38.855 | 1.00 | 45.16 |
| | ATOM | 4565 | O | WAT | W | 263 | 25.834 | 32.385 | -27.930 | 1.00 | 39.41 |
| 45 | ATOM | 4566 | O | WAT | W | 264 | 70.140 | -4.383 | 3.316 | 1.00 | 42.01 |
| | ATOM | 4567 | O | WAT | W | 265 | 17.686 | 28.637 | -27.597 | 1.00 | 36.50 |
| | ATOM | 4568 | O | WAT | W | 266 | 30.498 | 10.397 | 17.979 | 1.00 | 38.49 |
| | ATOM | 4569 | O | WAT | W | 267 | 41.552 | 17.448 | -14.793 | 1.00 | 45.70 |
| | ATOM | 4570 | O | WAT | W | 268 | 43.965 | -4.267 | 15.684 | 1.00 | 47.33 |
| 50 | ATOM | 4571 | O | WAT | W | 269 | 24.247 | 23.631 | -0.377 | 1.00 | 52.61 |
| | ATOM | 4572 | O | WAT | W | 270 | 39.439 | 16.949 | -2.045 | 1.00 | 40.49 |
| | ATOM | 4573 | O | WAT | W | 271 | 49.374 | 23.294 | 3.413 | 1.00 | 46.56 |
| | ATOM | 4574 | O | WAT | W | 272 | 39.872 | 8.421 | -18.197 | 1.00 | 45.41 |
| | ATOM | 4575 | O | WAT | W | 273 | 46.466 | -1.275 | 7.239 | 1.00 | 47.88 |
| 55 | ATOM | 4576 | O | WAT | W | 274 | 29.019 | 38.205 | -20.300 | 1.00 | 61.46 |
| | ATOM | 4577 | O | WAT | W | 275 | 69.375 | 1.409 | 13.444 | 1.00 | 43.48 |
| | ATOM | 4578 | O | WAT | W | 276 | 72.207 | 3.732 | 29.386 | 1.00 | 40.43 |
| | ATOM | 4579 | O | WAT | W | 277 | 39.712 | 37.170 | 0.051 | 1.00 | 39.08 |
| | ATOM | 4580 | O | WAT | W | 278 | 48.094 | -1.929 | 10.639 | 1.00 | 35.23 |
| 60 | ATOM | 4581 | O | WAT | W | 279 | 46.176 | -0.007 | 10.070 | 1.00 | 57.82 |
| | ATOM | 4582 | O | WAT | W | 280 | 34.060 | 14.226 | -7.694 | 1.00 | 47.69 |
| | ATOM | 4583 | O | WAT | W | 281 | 66.985 | -1.458 | 15.223 | 1.00 | 40.31 |
| | ATOM | 4584 | O | WAT | W | 282 | 69.909 | -11.226 | 6.382 | 1.00 | 54.99 |
| | ATOM | 4585 | O | WAT | W | 283 | 27.681 | 22.895 | 8.733 | 1.00 | 41.91 |
| 65 | ATOM | 4586 | O | WAT | W | 284 | 44.274 | -3.092 | 9.331 | 1.00 | 47.80 |
| | ATOM | 4587 | O | WAT | W | 285 | 35.726 | 14.777 | -5.459 | 1.00 | 63.96 |
| | ATOM | 4588 | O | WAT | W | 286 | 36.355 | 13.676 | -2.214 | 1.00 | 51.47 |
| | ATOM | 4589 | O | WAT | W | 287 | 45.262 | 7.207 | 17.415 | 1.00 | 54.68 |
| | ATOM | 4590 | O | WAT | W | 288 | 68.185 | 20.756 | 43.230 | 1.00 | 51.92 |
| 70 | ATOM | 4591 | O | WAT | W | 289 | 61.045 | 16.189 | 10.892 | 1.00 | 47.39 |
| | ATOM | 4592 | O | WAT | W | 290 | 37.948 | 29.641 | -14.217 | 1.00 | 51.54 |
| | ATOM | 4593 | O | WAT | W | 291 | 25.752 | 1.732 | 16.571 | 1.00 | 50.52 |
| | ATOM | 4594 | O | WAT | W | 292 | 21.651 | 4.509 | 5.878 | 1.00 | 55.37 |
| | ATOM | 4595 | O | WAT | W | 293 | 57.826 | 3.992 | 44.663 | 1.00 | 46.21 |
| | ATOM | 4596 | O | WAT | W | 294 | 66.103 | 19.731 | 40.130 | 1.00 | 39.58 |

-99-

| | | | | | | | | | | | |
|----|------|------|---|-----|---|-----|--------|---------|---------|------|-------|
| | ATOM | 4597 | O | WAT | W | 295 | 46.479 | -4.707 | 17.542 | 1.00 | 44.15 |
| | ATOM | 4598 | O | WAT | W | 296 | 71.219 | -3.422 | 0.474 | 1.00 | 42.17 |
| | ATOM | 4599 | O | WAT | W | 297 | 39.881 | 2.904 | 14.591 | 1.00 | 39.80 |
| 5 | ATOM | 4600 | O | WAT | W | 298 | 56.543 | 16.797 | 18.584 | 1.00 | 46.72 |
| | ATOM | 4601 | O | WAT | W | 299 | 61.789 | -18.999 | 2.206 | 1.00 | 57.02 |
| | ATOM | 4602 | O | WAT | W | 300 | 42.705 | 10.878 | -13.312 | 1.00 | 41.71 |
| | ATOM | 4603 | O | WAT | W | 301 | 69.432 | 7.509 | 6.399 | 1.00 | 56.46 |
| | ATOM | 4604 | O | WAT | W | 302 | 50.399 | 1.771 | -8.208 | 1.00 | 46.36 |
| | ATOM | 4605 | O | WAT | W | 303 | 80.707 | 8.597 | 32.436 | 1.00 | 57.84 |
| 10 | ATOM | 4606 | O | WAT | W | 304 | 35.950 | -3.190 | -6.617 | 1.00 | 47.01 |
| | ATOM | 4607 | O | WAT | W | 305 | 63.191 | 13.663 | 10.338 | 1.00 | 47.69 |
| | ATOM | 4608 | O | WAT | W | 306 | 32.746 | 17.045 | 16.882 | 1.00 | 38.37 |
| | ATOM | 4609 | O | WAT | W | 307 | 55.795 | 22.081 | -3.121 | 1.00 | 45.39 |
| | ATOM | 4610 | O | WAT | W | 308 | 52.917 | -15.266 | -5.084 | 1.00 | 58.04 |
| 15 | ATOM | 4611 | O | WAT | W | 309 | 32.990 | 20.281 | -2.705 | 1.00 | 41.15 |
| | ATOM | 4612 | O | WAT | W | 310 | 65.221 | -0.521 | 13.373 | 1.00 | 50.04 |
| | ATOM | 4613 | O | WAT | W | 311 | 31.445 | 8.146 | -16.640 | 1.00 | 47.12 |
| | ATOM | 4614 | O | WAT | W | 312 | 70.526 | -1.084 | -1.047 | 1.00 | 43.90 |
| | ATOM | 4615 | O | WAT | W | 313 | 67.588 | -6.363 | 21.900 | 1.00 | 57.15 |
| 20 | ATOM | 4616 | O | WAT | W | 314 | 66.096 | -4.686 | 20.242 | 1.00 | 69.24 |
| | ATOM | 4617 | O | WAT | W | 315 | 47.292 | 23.337 | 13.967 | 1.00 | 42.45 |
| | ATOM | 4618 | O | WAT | W | 316 | 77.697 | -6.690 | 46.864 | 1.00 | 61.61 |
| | ATOM | 4619 | O | WAT | W | 317 | 57.134 | 18.189 | -19.802 | 1.00 | 61.48 |
| | ATOM | 4620 | O | WAT | W | 318 | 56.615 | 6.099 | -16.259 | 1.00 | 55.28 |
| 25 | ATOM | 4621 | O | WAT | W | 319 | 70.759 | 17.127 | 50.284 | 1.00 | 46.60 |
| | ATOM | 4622 | O | WAT | W | 320 | 72.021 | -17.283 | 5.694 | 1.00 | 53.07 |
| | ATOM | 4623 | O | WAT | W | 321 | 23.729 | 4.269 | -4.449 | 1.00 | 58.06 |
| | ATOM | 4624 | O | WAT | W | 322 | 22.138 | 20.117 | -24.492 | 1.00 | 37.83 |
| | ATOM | 4625 | O | WAT | W | 323 | 40.526 | 13.448 | -0.063 | 1.00 | 54.95 |
| 30 | ATOM | 4626 | O | WAT | W | 324 | 28.034 | -4.586 | 23.421 | 1.00 | 50.98 |
| | ATOM | 4627 | O | WAT | W | 325 | 38.920 | 16.623 | -33.391 | 1.00 | 53.48 |
| | ATOM | 4628 | O | WAT | W | 326 | 77.040 | -7.476 | 27.616 | 1.00 | 73.56 |
| | ATOM | 4629 | O | WAT | W | 327 | 68.678 | -0.075 | 28.998 | 1.00 | 51.90 |
| | ATOM | 4630 | O | WAT | W | 328 | 46.505 | 7.743 | -11.664 | 1.00 | 43.38 |
| 35 | ATOM | 4631 | O | WAT | W | 329 | 43.657 | 18.299 | -3.514 | 1.00 | 20.00 |
| | ATOM | 4632 | O | WAT | W | 330 | 40.596 | 13.269 | -4.354 | 1.00 | 20.00 |
| | ATOM | 4633 | O | WAT | W | 331 | 66.428 | -1.404 | 17.847 | 1.00 | 20.00 |
| | ATOM | 4634 | O | WAT | W | 332 | 41.584 | 19.897 | -1.703 | 1.00 | 20.00 |
| | ATOM | 4635 | O | WAT | W | 333 | 41.694 | 22.971 | -4.274 | 1.00 | 20.00 |
| 40 | ATOM | 4636 | O | WAT | W | 334 | 67.997 | 3.764 | 15.541 | 1.00 | 20.00 |
| | ATOM | 4637 | O | WAT | W | 335 | 60.537 | 18.286 | 2.068 | 1.00 | 20.00 |
| | ATOM | 4638 | O | WAT | W | 336 | 56.447 | 20.428 | 10.716 | 1.00 | 20.00 |
| | ATOM | 4639 | O | WAT | W | 337 | 55.557 | 22.546 | 9.246 | 1.00 | 20.00 |
| | ATOM | 4640 | O | WAT | W | 338 | 58.179 | 16.183 | -0.749 | 1.00 | 20.00 |
| 45 | ATOM | 4641 | O | WAT | W | 339 | 58.887 | 16.112 | -3.916 | 1.00 | 20.00 |
| | ATOM | 4642 | O | WAT | W | 340 | 63.509 | 11.351 | 2.806 | 1.00 | 20.00 |
| | ATOM | 4643 | O | WAT | W | 341 | 62.716 | 14.296 | 1.151 | 1.00 | 20.00 |
| | ATOM | 4644 | O | WAT | W | 342 | 39.563 | -4.272 | 12.971 | 1.00 | 20.00 |
| | ATOM | 4645 | O | WAT | W | 343 | 39.743 | -6.346 | 11.592 | 1.00 | 20.00 |
| 50 | ATOM | 4646 | O | WAT | W | 344 | 44.345 | -8.782 | 9.282 | 1.00 | 20.00 |
| | ATOM | 4647 | O | WAT | W | 345 | 38.126 | -6.949 | 4.925 | 1.00 | 20.00 |
| | ATOM | 4648 | O | WAT | W | 346 | 41.558 | -9.568 | 2.423 | 1.00 | 20.00 |
| | ATOM | 4649 | O | WAT | W | 347 | 46.133 | -8.864 | -1.132 | 1.00 | 20.00 |
| | ATOM | 4650 | O | WAT | W | 348 | 42.431 | 12.582 | 19.513 | 1.00 | 20.00 |
| 55 | ATOM | 4651 | O | WAT | W | 349 | 39.817 | 3.709 | 21.589 | 1.00 | 20.00 |
| | ATOM | 4652 | O | WAT | W | 350 | 40.535 | 5.544 | 20.119 | 1.00 | 20.00 |
| | ATOM | 4653 | O | WAT | W | 351 | 41.467 | 8.090 | 20.981 | 1.00 | 20.00 |
| | ATOM | 4654 | O | WAT | W | 352 | 61.469 | 16.879 | -5.628 | 1.00 | 20.00 |
| | ATOM | 4655 | O | WAT | W | 353 | 57.522 | 13.280 | -9.676 | 1.00 | 20.00 |
| 60 | ATOM | 4656 | O | WAT | W | 354 | 57.275 | 9.042 | -5.426 | 1.00 | 20.00 |
| | ATOM | 4657 | O | WAT | W | 355 | 59.327 | 5.417 | -6.085 | 1.00 | 20.00 |
| | ATOM | 4658 | O | WAT | W | 356 | 52.962 | -4.323 | -3.179 | 1.00 | 20.00 |
| | ATOM | 4659 | O | WAT | W | 357 | 36.344 | -8.909 | 7.979 | 1.00 | 20.00 |
| | ATOM | 4660 | O | WAT | W | 358 | 42.391 | 30.320 | -15.418 | 1.00 | 20.00 |
| 65 | ATOM | 4661 | O | WAT | W | 359 | 52.354 | 18.876 | -21.657 | 1.00 | 20.00 |
| | ATOM | 4662 | O | WAT | W | 360 | 85.510 | 2.059 | 39.934 | 1.00 | 20.00 |
| | ATOM | 4663 | O | WAT | W | 361 | 86.895 | 4.068 | 37.822 | 1.00 | 20.00 |
| | ATOM | 4664 | O | WAT | W | 362 | 81.610 | 8.015 | 30.106 | 1.00 | 20.00 |
| | ATOM | 4665 | O | WAT | W | 363 | 81.600 | 7.773 | 49.392 | 1.00 | 20.00 |
| 70 | ATOM | 4666 | O | WAT | W | 364 | 76.414 | 9.988 | 52.505 | 1.00 | 20.00 |
| | ATOM | 4667 | O | WAT | W | 365 | 67.897 | 8.778 | 49.346 | 1.00 | 20.00 |
| | ATOM | 4668 | O | WAT | W | 366 | 63.858 | 2.436 | 46.800 | 1.00 | 20.00 |
| | ATOM | 4669 | O | WAT | W | 367 | 71.953 | 1.096 | 48.138 | 1.00 | 20.00 |
| | ATOM | 4670 | O | WAT | W | 368 | 89.873 | -11.648 | 35.808 | 1.00 | 20.00 |

-100-

| | | | | | | | | | | |
|----|------|------|---|-------|-----|--------|---------|--------|-------|-------|
| | ATOM | 4671 | O | WAT W | 369 | 88.460 | -12.813 | 38.004 | -1.00 | 20.00 |
| | ATOM | 4672 | O | WAT W | 370 | 91.761 | -9.669 | 35.928 | 1.00 | 20.00 |
| | ATOM | 4673 | O | WAT W | 371 | 88.580 | -15.367 | 38.475 | 1.00 | 20.00 |
| 5 | ATOM | 4674 | O | WAT W | 372 | 76.861 | -9.543 | 44.348 | 1.00 | 20.00 |
| | ATOM | 4675 | O | WAT W | 373 | 74.471 | -6.743 | 45.210 | 1.00 | 20.00 |
| | ATOM | 4676 | O | WAT W | 374 | 79.402 | -2.424 | 46.754 | 1.00 | 20.00 |
| | ATOM | 4677 | O | WAT W | 375 | 75.647 | -0.122 | 49.778 | 1.00 | 20.00 |
| | ATOM | 4678 | O | WAT W | 376 | 77.752 | 1.584 | 49.411 | 1.00 | 20.00 |
| 10 | ATOM | 4679 | O | WAT W | 377 | 37.468 | -4.589 | 21.373 | 1.00 | 20.00 |
| | ATOM | 4680 | O | WAT W | 378 | 45.334 | -7.735 | 21.716 | 1.00 | 20.00 |
| | ATOM | 4681 | O | WAT W | 379 | 46.136 | -5.299 | 22.588 | 1.00 | 20.00 |
| | ATOM | 4682 | O | WAT W | 380 | 43.144 | -7.232 | 20.423 | 1.00 | 20.00 |
| | ATOM | 4683 | O | WAT W | 381 | 42.129 | -4.775 | 20.988 | 1.00 | 20.00 |
| 15 | ATOM | 4684 | O | WAT W | 382 | 47.659 | -14.000 | 24.499 | 1.00 | 20.00 |
| | ATOM | 4685 | O | WAT W | 383 | 41.892 | -6.834 | 15.632 | 1.00 | 20.00 |
| | ATOM | 4686 | O | WAT W | 384 | 42.961 | -8.398 | 13.868 | 1.00 | 20.00 |

Table 2

Composition of defined minimal culture medium for selenium-containing PS. All components were filter-sterilized through 0.22µm filters, except where indicated.

| Compound | Stock conc. | Volume | Comments |
|------------------------|---------------------|--------|--|
| M9 medium ^a | 1 | 250 ml | Autoclaved. |
| MgSO ₄ | 1 M | 250 µl | Autoclaved separately from M9 medium to avoid precipitation. |
| D-glucose | 4% w/v | 25 ml | Not autoclaved, since that caused glucose to caramelize (yellow colour); filter sterilized instead. |
| Thiamine | 0.5% w/v | 25 µl | Prepared stock and stored at -20°C; since repeated cycles of freeze and thaw do not damage it. |
| FeSO ₄ | 4.2 g/l | 250 µl | Prepared stock and stored at -20°C, to prevent oxidation. |
| Ampicillin | 100 mg/ml | 250 µl | Filter sterilized and stored as aliquots – cycles of freeze and thaw were avoided. |
| IPTG | 70 mg/ml | 250 µl | |
| L-arginine | 2.53% w/v | 5 ml | Supplemented for AT1371 deficiency; prepared together as single stock. |
| L-histidine | 0.31% w/v | | |
| L-proline | 4.6% w/v | | |
| Adenine | 1.35% w/v | | |
| L-lysine | 12.5 g/l | 2 ml | Cocktail for methionine pathway inhibition; prepared as one stock. Final concentrations were 100 and 50 mg/l respectively. |
| L-phenylalanine | 12.5 g/l | | |
| L-threonine | 12.5 g/l | | |
| L-isoleucine | 6.25 g/l | | |
| L-leucine | 6.25 g/l | | |
| L-valine | 6.25 g/l | | |
| L-seleno-methionine | Final conc: 50 mg/l | - | No need to sterilise, to minimise risk of oxidation. Dissolved in water directly in bottle in which supplied, then added. |

^a Sambrook, J., Fritsch, E. F. & Maniatis, T. (1989). *Molecular cloning: a laboratory manual*, 2nd ed. Cold Spring Harbour Laboratory Press, Cold Spring Harbor, N.Y.

-102-

Table 3

| | | |
|--|---|--|
| <i>Crystallographic refinement</i> | | |
| No. reflexions (test set) | 77 294 (4062) | Test set is excluded from refinement for cross-validation |
| No. restraints | 15 730 | Restraints in TNT with a weight assigned |
| No. parameters | 20 236 | |
| Weight for geom. restraints (TNT) | 3 | |
| <i>Final model parameters</i> | | |
| Residues | 566 | |
| Hetero | 1 Tris, 2 ethanediol | |
| No. water molecules | 622 | |
| No. non-hydrogen atoms | 5059 | |
| Resolution range (Å) | 45 - 1.7 | |
| <i>Refinement convergence</i> | | |
| R_{free} | 24.9 | R_{factor} calculated using test reflexions |
| R_{factor} | 22.6 | $R_{factor} = \sum_h F_{obs} - F_{calc} / \sum_h F_{obs} $, w/o test reflexions. |
| DDQ (score, ranking) | UFO | "Unassigned positive Feature left-Over score" |
| | DDQ-R | Ratio of Shift and Water peak contributions. |
| Average B -factor, | | |
| subunit A (Å ²) | 33.9 | |
| subunit B (Å ²) | 36.4 | |
| waters (Å ²) | 47.8 | |
| Wilson distribution B_{factor} (Å ²) | 28.0 | |
| <i>Model quality</i> | | |
| Ramachandran plot | % residues in most favoured region | 92.2 |
| | % residues in generously-allowed region | 7.4 |
| | No. residues in disallowed region | 0 |
| Rms deviation from ideal | Covalent bond lengths (Å) | 0.018 |
| ("root mean square") | Bond angles (°) | 1.41 |
| | Planar groups (Å) | 0.007 |
| Procheck criteria | % bond lengths outside expected limits | 2.6 |
| | % bond angles outside expected limits | 3.1 |
| | % planar groups outside expected limits | 1.0 |
| WhatCheck criteria | No. unsaturated H-bonds | 2 |
| | No. residues in unusual environments | 14 |

-103-

Table 4

Residues lining the PS binding pockets

| | |
|----|--------|
| 5 | Val27 |
| | Pro28 |
| | Thr29 |
| | Met30 |
| | Gly31 |
| 10 | Asn32 |
| | Leu33 |
| | His34 |
| | Asp35 |
| | Gly36 |
| 15 | His37 |
| | Lys39 |
| | Leu40 |
| | Ser54 |
| | Phe56 |
| 20 | Asn58 |
| | Gln61 |
| | Phe62 |
| | Tyr71 |
| | Phe91 |
| 25 | Pro93 |
| | Ile98 |
| | Leu118 |
| | Glu119 |
| | His126 |
| 30 | Phe127 |
| | Val130 |
| | Ile133 |
| | Val134 |
| | Lys136 |
| 35 | Leu137 |
| | Leu140 |
| | Cys147 |
| | Phe148 |
| | Gly149 |
| 40 | Glu150 |
| | Lys151 |
| | Asp152 |
| | Phe153 |
| | Gln154 |
| 45 | Gln155 |
| | Leu156 |
| | Ile159 |
| | Ile172 |
| | Val175 |
| 50 | Pro176 |
| | Ile177 |
| | Met178 |
| | Arg179 |
| | Leu184 |
| 55 | Ala185 |
| | Leu186 |
| | Ser187 |
| | Ser188 |
| | Arg189 |
| 60 | Asn190 |
| | Asp242 |
| | Leu251 |
| | Leu264 |
| | Val265 |
| 65 | Ala266 |
| | Arg273 |
| | Leu274 |
| | Ile275 |
| | Asp276 |
| 70 | Asn277 |

Claims:

1. A crystal of pantothenate synthetase (PS) having a monoclinic space group $P2_1$ and unit cell dimensions of $a = 66.0 \pm 0.2 \text{ \AA}$, $b = 78.1 \pm 0.2 \text{ \AA}$, $c = 77.1 \pm 0.2 \text{ \AA}$ and $\beta = 103.7 \pm 0.2^\circ$.
2. A crystal of PS having the three dimensional atomic coordinates of Table 1.
3. A method for crystallizing a selenium atom PS derivative which comprises producing PS by recombinant production in a bacterial host in the presence of selenomethionine, recovering a selenium atom PS derivative from the host and growing crystals from the recovered selenium atom PS derivative.
4. A computer-based method of rational drug design which comprises:
 - providing the structure of the PS as defined by the coordinates of Table 1;
 - providing the structure of a candidate modulator molecule; and
 - fitting the structure of the candidate modulator molecule to the structure of the PS of Table 1.
5. A computer-based method of rational drug design which comprises:
 - providing the coordinates of at least two atoms of the PS of Table 1;
 - providing the structure of a candidate modulator molecule; and
 - fitting the structure of the candidate modulator molecule to the provided coordinates of the PS.
6. A computer-based method of rational drug design which comprises:

-105-

providing the coordinates of at least a sub-domain of the PS;

providing the structure of a candidate modulator molecule; and

5 fitting the structure of the candidate modulator molecule to the coordinates of the PS sub-domain provided.

7. The method of any one of claims 4 to 6 which further comprises the steps of:

10 obtaining or synthesising the candidate modulator; and contacting the candidate modulator with PS to determine the ability of the candidate modulator to interact with PS.

8. The method of any one of claims 4 to 6 which further comprises the steps of:

15 obtaining or synthesising said candidate modulator; forming a complex of PS and said potential modulator; and analysing said complex by X-ray crystallography to determine the ability of said candidate modulator to interact
20 with PS.

9. A compound having a chemical structure selected using the method of any one of claims 4 to 6, said compound being an inhibitor of PS.

25

10. A computer readable medium with either (a) atomic data according to Table 1 recorded thereon, said data defining the three-dimensional structure of PS or at least one sub-domain thereof or (b) structure factor data for PS recorded thereon,
30 the structure factor data being derivable from the atomic coordinate data of Table 1.

11. A computer system, intended to generate structures and/or perform rational drug design for PS or complexes of PS with a

-106-

- potential modulator, the system containing either (a) atomic coordinate data according to Table 1, said data defining the three-dimensional structure of PS or at least one sub-domain thereof or (b) structure factor data for PS, said structure factor data being derivable from the atomic coordinate data of Table 1.
- 5

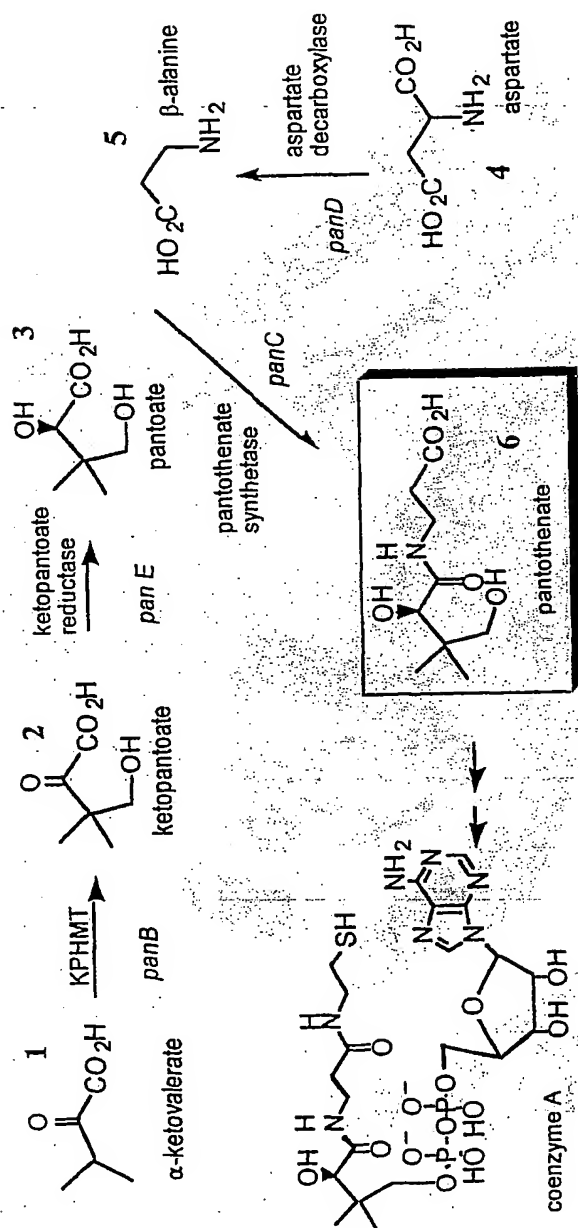


Fig. 1



Fig. 2a

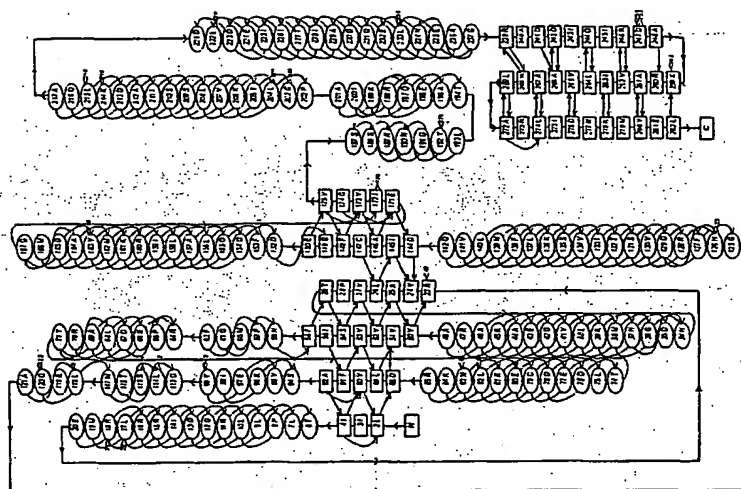


Fig. 2c

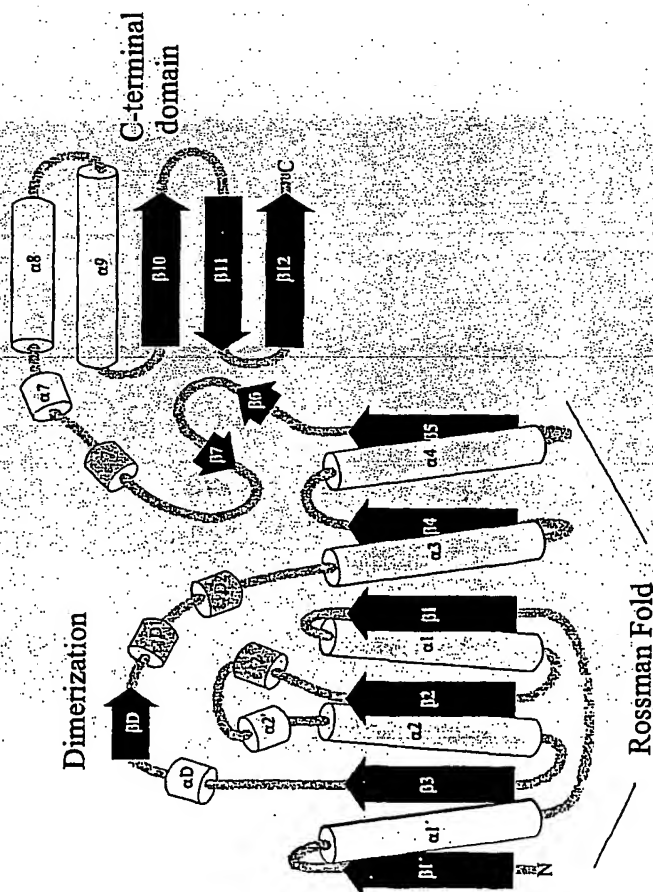


Fig. 2b

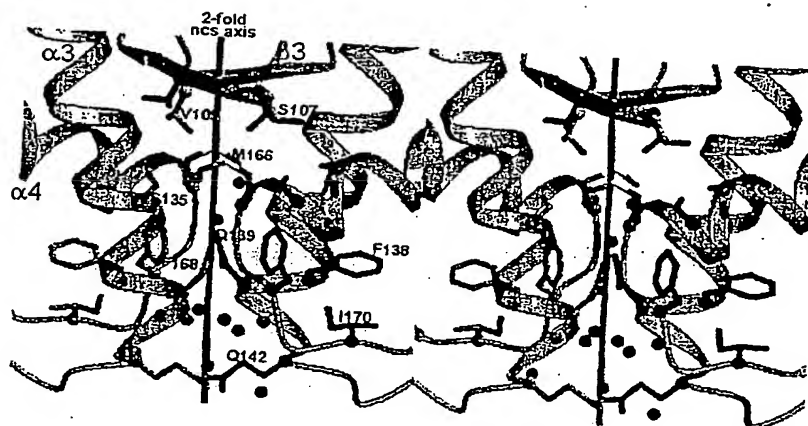


Fig. 3

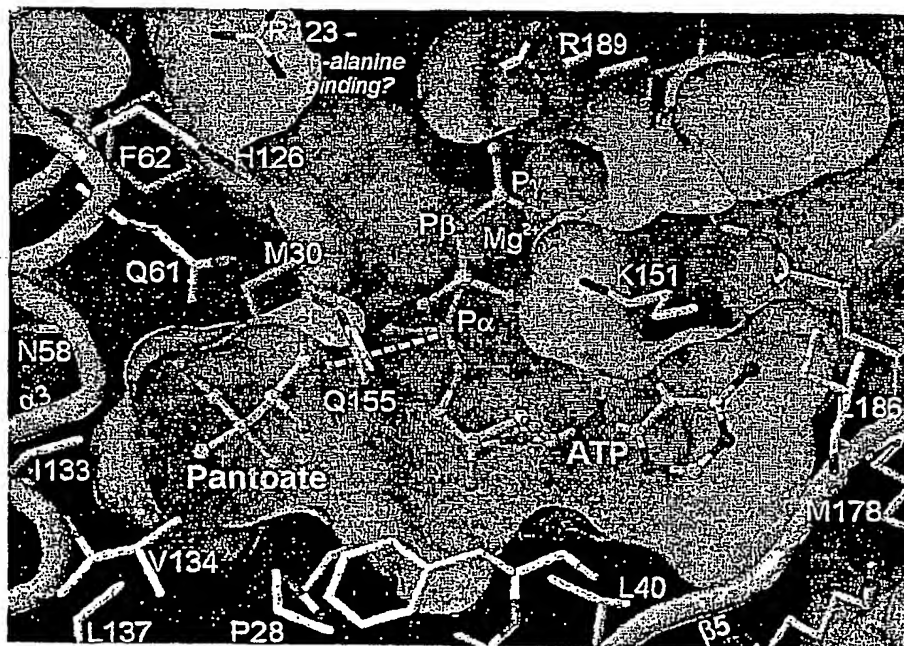


Fig. 4

INTERNATIONAL SEARCH REPORT

Int. Application No

PCT/GB 01/04067

A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C12N9/00 G06F17/50

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C12N G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, BIOSIS, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category * | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|------------|--|-----------------------|
| P, X | <p>DELFT ET AL: "The crystal structure of E. coli pantothenate synthetase confirms it as a member of the cytidylyltransferase superfamily" STRUCTURE, vol. 9, May 2001 (2001-05), pages 439-450, XP002187263</p> <p>* See page 441 (Table 1), page 442 (Figure 2), page 448 (Experimental Procedures) and page 450 (footnote -> PDB = 1IH0; release date: 30.05.2001 *</p> <p style="text-align: center;">-/-</p> | 1-8, 10, 11 |

☒ Further documents are listed in the continuation of box C.☐ Patent family members are listed in annex.

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Date of the actual completion of the international search

14 January 2002

Date of mailing of the international search report

04/02/2002

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Authorized officer

Korsner, S-E

INTERNATIONAL SEARCH REPORT

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| Category * | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|------------|---|-----------------------|
| A | <p>QORONFLEH ET AL: "Production of selenomethionine-labeled recombinant human neutrophil collagenase in Escherichia coli"</p> <p>JOURNAL OF BIOTECHNOLOGY, ELSEVIER SCIENCE PUBLISHERS, AMSTERDAM, NL, vol. 39, no. 2, 15 April 1995 (1995-04-15), pages 119-128, XP004036977</p> <p>ISSN: 0168-1656</p> <p>* See pages 119-120</p> <p>(Introduction/Selenomethionine/MAD) *</p> <p>---</p> | 1-8,10, 11 |
| A | <p>SHAO ET AL: "Accessibility of selenomethionine proteins by total chemical synthesis: structural studies of human herpesvirus-8 MIP-II"</p> <p>FEBS LETTERS, ELSEVIER SCIENCE PUBLISHERS, AMSTERDAM, NL, vol. 441, no. 1, 11 December 1998 (1998-12-11), pages 77-82, XP004258875</p> <p>ISSN: 0014-5793</p> <p>* See page 77 (Introduction) *</p> <p>---</p> | 1-8,10, 11 |
| T | <p>JHOTI H: "High-throughput structural proteomics using x-rays"</p> <p>TRENDS IN BIOTECHNOLOGY, ELSEVIER PUBLICATIONS, CAMBRIDGE, GB, vol. 19, no. 10, 1 October 2001 (2001-10-01), pages S67-S71, XP004310381</p> <p>ISSN: 0167-7799</p> <p>* See pages S69-S70 (Structure to drug lead) *</p> <p>-----</p> | 1-8,10, 11 |

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 9

Present Claim 9 relates to undefined compounds that may be obtained by using the method of Claims 4-6. This is merely a desideratum, and no such compounds have been identified by the Applicant. Since they are undefined, it is not possible to carry out a meaningful search.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.